



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:45 AM UTC

PDB ID : 8FR8 / pdb_00008fr8
EMDB ID : EMD-29397
Title : Structure of Mycobacterium smegmatis Rsh bound to a 70S translation initiation complex
Authors : Majumdar, S.; Sharma, M.R.; Manjari, S.R.; Banavali, N.K.; Agrawal, R.K.
Deposited on : 2023-01-06
Resolution : 2.76 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

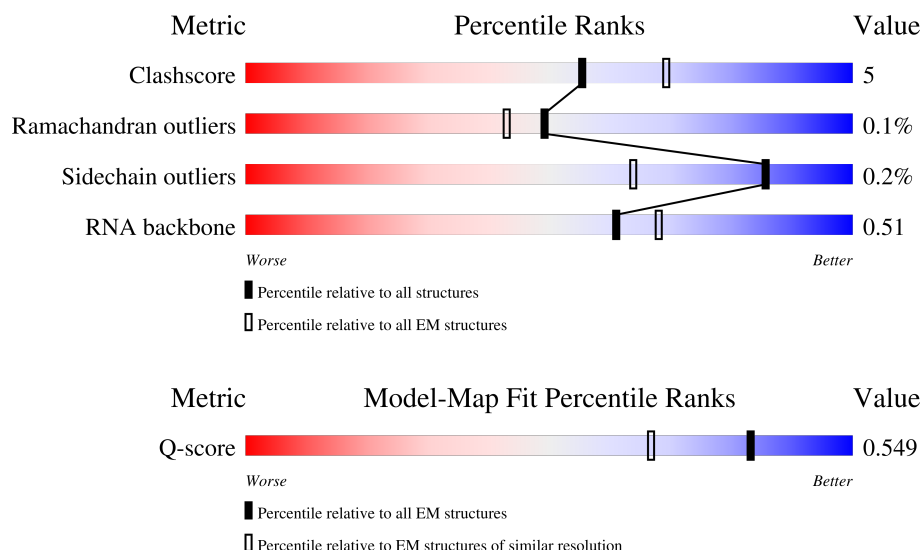
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.76 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.



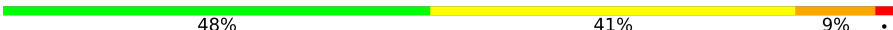
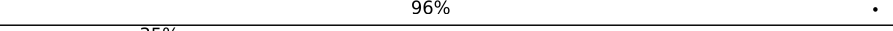
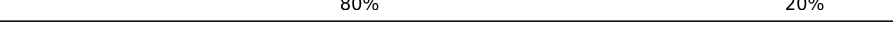
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10642 (2.26 - 3.26)

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

Mol	Chain	Length	Quality of chain
1	c	53	
2	y	77	
3	E	77	

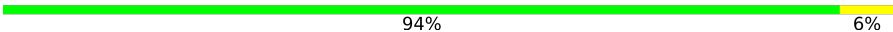
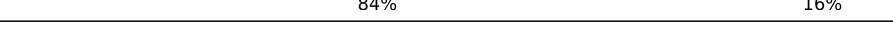
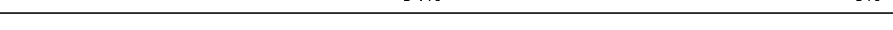
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Mol	Chain	Length	Quality of chain
4	d	82	
5	B	118	
6	j	116	
7	N	136	
8	3	23	
9	A	3119	
10	K	275	
11	L	214	
12	M	209	
13	O	182	
14	P	176	
15	Q	151	
16	R	126	
17	S	133	
18	T	146	
19	U	122	
20	V	145	
21	J	118	
22	D	126	
23	C	113	
24	W	124	
25	X	100	
26	Y	114	
27	Z	97	
28	1	105	

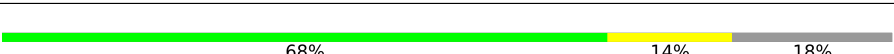
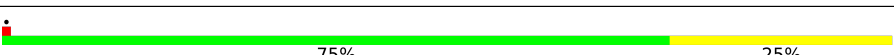
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Mol	Chain	Length	Quality of chain
29	2	192	 76%18%6%
30	4	79	 94%6%
31	6	64	 91%9%
32	7	59	 78%22%
33	8	54	 91%9%
34	0	46	 87%13%
35	x	63	 87%13%
36	F	37	 78%22%
37	a	1511	 68%28%. .
38	b	32	 88%12%
39	G	208	 82%17%. .
40	e	200	 76%24%
41	f	180	 89%11%. .
42	g	96	 84%16%
43	h	155	 90%10%
44	i	131	 86%14%
45	k	126	 88%12%
46	l	99	 74%26%
47	m	115	 94%6%
48	n	122	 77%23%
49	p	88	 82%18%
50	q	113	 82%18%. .
51	r	94	 86%14%
52	t	85	 92%8%
53	u	228	 79%21%

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Mol	Chain	Length	Quality of chain
54	v	20	
55	I	797	
56	H	82	
57	o	84	
58	9	100	

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 152820 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L33 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	c	49	Total	C	N	O	0	0
			423	263	89	71		

- Molecule 2 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	y	76	Total	C	N	O	S	0	0
			605	368	131	104	2		

- Molecule 3 is a RNA chain called fMet tRNA (77-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	77	Total	C	N	O	P	0	0
			1642	731	293	541	77		

- Molecule 4 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	82	Total	C	N	O	S	0	0
			662	425	124	112	1		

- Molecule 5 is a RNA chain called 5S rRNA (118-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	118	Total	C	N	O	P	0	0
			2522	1126	468	810	118		

- Molecule 6 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	j	116	Total	C	N	O	S	0	0
			935	572	191	169	3		

- Molecule 7 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	136	Total	C	N	O	S	0	0
			1092	690	213	187	2		

- Molecule 8 is a protein called 50S ribosomal protein eL31.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	3	23	Total	C	N	O	0	0
			189	111	50	28		

- Molecule 9 is a RNA chain called 23S rRNA (3119-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	3119	Total	C	N	O	P	0	0
			66981	29854	12313	21695	3119		

- Molecule 10 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	275	Total	C	N	O	S	0	0
			2110	1298	438	370	4		

- Molecule 11 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	214	Total	C	N	O	S	0	0
			1587	982	310	290	5		

- Molecule 12 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	209	Total	C	N	O	S	0	0
			1569	969	295	303	2		

- Molecule 13 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	182	Total	C	N	O	S	0	0
			1445	907	271	261	6		

- Molecule 14 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	176	Total	C	N	O	S	0	0
			1348	845	249	253	1		

- Molecule 15 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	151	Total	C	N	O	S	0	0
			1018	635	188	194	1		

- Molecule 16 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	126	Total	C	N	O	S	0	0
			918	580	156	180	2		

- Molecule 17 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	133	Total	C	N	O	S	0	0
			990	625	175	187	3		

- Molecule 18 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	146	Total	C	N	O	S	0	0
			1130	722	207	200	1		

- Molecule 19 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	122	Total	C	N	O	S	0	0
			938	586	179	170	3		

- Molecule 20 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	145	Total	C	N	O	S	0	0
			1078	676	205	194	3		

- Molecule 21 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	J	118	Total	C	N	O	S	0	0
			928	583	180	163	2		

- Molecule 22 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	D	126	Total	C	N	O		0	0
			956	586	199	171			

- Molecule 23 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	C	113	Total	C	N	O	S	0	0
			907	570	171	165	1		

- Molecule 24 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	124	Total	C	N	O		0	0
			988	613	203	172			

- Molecule 25 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	100	Total	C	N	O		0	0
			754	478	137	139			

- Molecule 26 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	114	Total	C	N	O		0	0
			873	543	171	159			

- Molecule 27 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	97	Total	C	N	O		0	0
			756	479	138	139			

- Molecule 28 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1	97	Total	C	N	O	S	0	0
			732	456	137	137	2		

- Molecule 29 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2	180	Total	C	N	O		0	0
			1347	833	243	271			

- Molecule 30 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4	79	Total	C	N	O		0	0
			586	361	123	102			

- Molecule 31 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	6	64	Total	C	N	O	S	0	0
			531	324	103	103	1		

- Molecule 32 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	7	59	Total	C	N	O		0	0
			474	292	95	87			

- Molecule 33 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	8	54	Total	C	N	O	S	0	0
			423	260	93	69	1		

- Molecule 34 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	0	46	Total	C	N	O	S	0	0
			377	225	97	54	1		

- Molecule 35 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	x	63	Total	C	N	O	0	0
			502	302	115	85		

- Molecule 36 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	F	37	Total	C	N	O	S	0	0
			299	181	66	47	5		

- Molecule 37 is a RNA chain called 16S rRNA (1511-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
37	a	1511	Total	C	N	O	P	0	0
			32439	14448	5930	10550	1511		

- Molecule 38 is a protein called 30S ribosomal protein S22.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	b	32	Total	C	N	O	S	0	0
			280	172	71	36	1		

- Molecule 39 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	G	208	Total	C	N	O	S	0	0
			1660	1036	322	298	4		

- Molecule 40 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	e	200	Total	C	N	O	S	0	0
			1641	1028	316	295	2		

- Molecule 41 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	f	180	Total	C	N	O	S	0	0
			1296	812	245	235	4		

- Molecule 42 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	g	96	Total	C	N	O	S	0	0
			771	486	138	145	2		

- Molecule 43 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	h	155	Total	C	N	O	S	0	0
			1232	768	241	221	2		

- Molecule 44 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	i	131	Total	C	N	O	S	0	0
			1010	633	189	187	1		

- Molecule 45 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	k	126	Total	C	N	O	S	0	0
			994	630	194	170			

- Molecule 46 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	l	99	Total	C	N	O	S	0	0
			788	495	146	144	3		

- Molecule 47 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	m	115	Total	C	N	O	S	0	0
			855	528	170	156	1		

- Molecule 48 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	n	122	Total	C	N	O	S	0	0
			958	594	197	165	2		

- Molecule 49 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	p	88	Total	C	N	O	0	0
			720	449	147	124		

- Molecule 50 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	q	113	Total	C	N	O	0	0
			891	570	162	159		

- Molecule 51 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	94	Total	C	N	O	S	0	0
			748	469	142	135	2		

- Molecule 52 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	t	85	Total	C	N	O	0	0
			660	402	139	119		

- Molecule 53 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	u	228	Total	C	N	O	S	0	0
			1793	1132	322	330	9		

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	v	18	Total	C	N	O	P	0	0
			388	175	76	120	17		

- Molecule 55 is a protein called GTP pyrophosphokinase RelA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	I	150	Total	C	N	O	S	0	0
			1126	700	200	221	5		

- Molecule 56 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	H	75	Total	C	N	O	S	0	0
			593	379	103	110	1		

- Molecule 57 is a protein called 30S ribosomal protein S18 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	o	69	Total	C	N	O	S	0	0
			543	338	107	96	2		

- Molecule 58 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	9	100	Total	C	N	O	S	0	0
			819	497	183	138	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: 50S ribosomal protein L33 2

Chain c: 



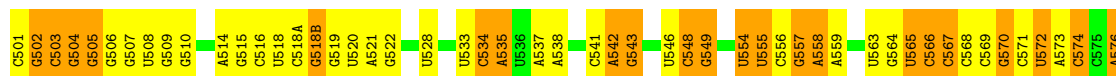
• Molecule 2: 50S ribosomal protein L28

Chain y: 



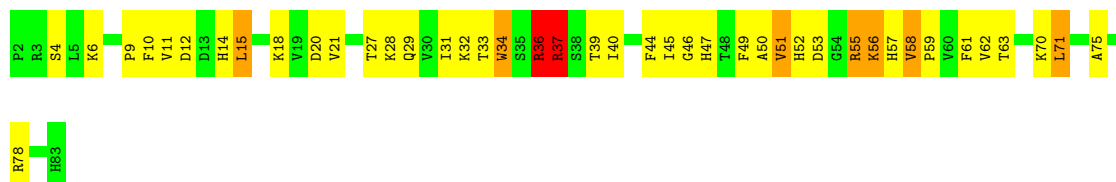
• Molecule 3: fMet tRNA (77-MER)

Chain E: 



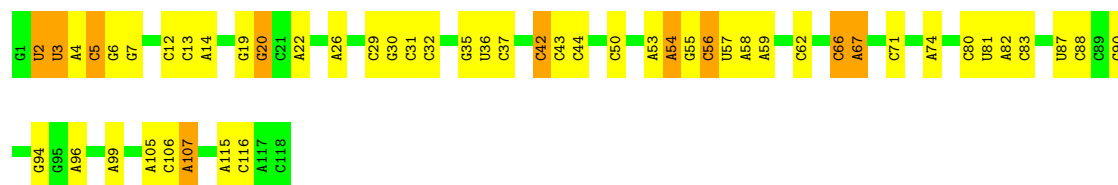
• Molecule 4: 30S ribosomal protein S19

Chain d: 



• Molecule 5: 5S rRNA (118-MER)

Chain B: 



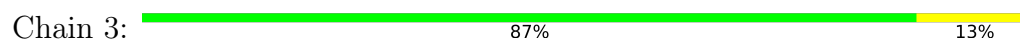
- Molecule 6: 30S ribosomal protein S13



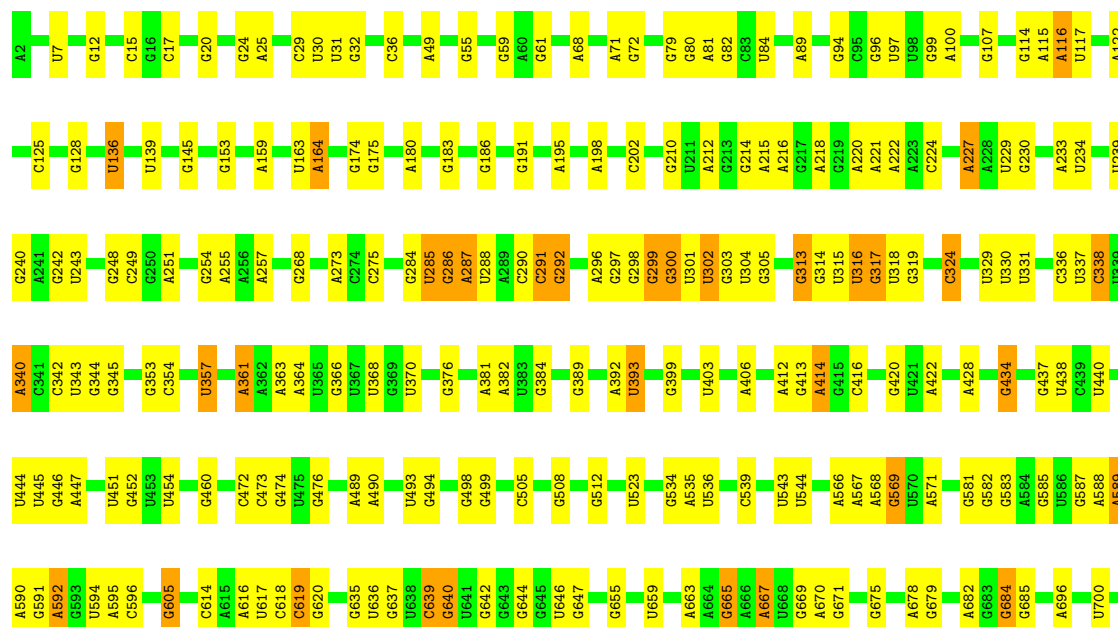
- Molecule 7: 50S ribosomal protein L16



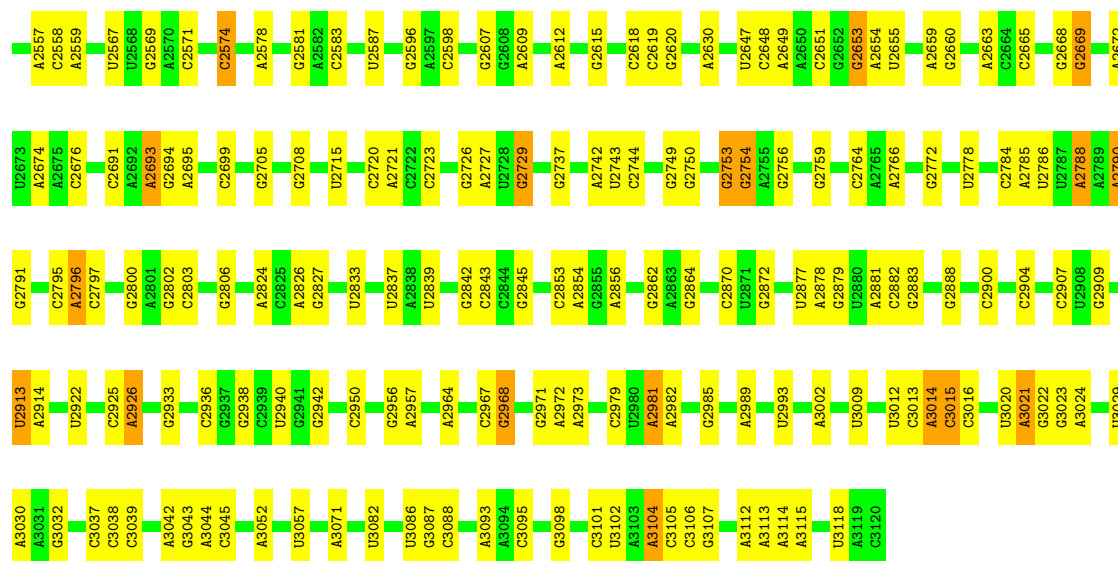
- Molecule 8: 50S ribosomal protein eL31



- Molecule 9: 23S rRNA (3119-MER)

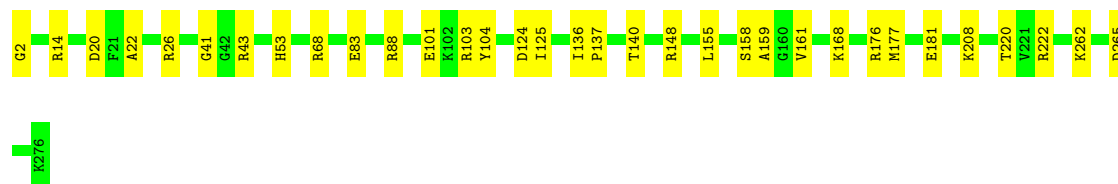


A2434	U2355	C2345	G2129	A1985	A1789	G1636	A1552	G1458	C1268	A1185	G1078	G874	G832	G706
U2435	G2356	U2246	G2130	A1974	C1797	A1639	C1553	U1428	C1269	G1186	G1085	G874	G838	G707
A2436	A2357	A2255	A2137	A1975	U1798	G1639	U1554	C1441	A1187	A1188	C1086	A978	U839	U709
G2441	G2358	G2256	A2138	A1981	U1641	U1640	A1556	G1456	G1189	G979	G879	C845	U714	
G2446	C2360	G2257	U2139	U1981	A1803	A1648	A1563	C1465	U1291	C1190	G1092	U981		
G2447	C2361	G2259	U2140	A1990	G1804	C1649	A1564	C1466	G1192	A1191	A101	A982	A849	A721
A2449	C2362	G2263	U2141	A1991	C1813	C1649	A1565	U1467	C1193	G1104	G1102	G985	A858	G722
U2457	A2365	C2267	A2151	U1992	G1825	G1658	A1566	U1470	G1304	C1104	C1103	G985	G859	G723
G2462	G2367	G2152	G2153	A2008	C1826	U1675	C1567	G1470	G1197	C1105	C1105	G990	G860	G724
G2463	C2368	G2154	G2154	G2016	A1827	G1676	C1571	A1474	U1200	A1106	G1107	G993	U861	A725
A2470	C2369	A2160	A2160	C2017	A1828	A1679	G1572	A1474	G1201	A1108	A1108	A994	U862	G728
G2471	A2370	G2178	G2178	C2018	A1834	U1681	U1573	G1479	A1202	U1109	G1109	U995	G863	C729
U2473	U2372	U2163	U2163	A2019	G1840	G1688	G1574	C1481	A1203	C1110	G1110	G996	U868	A731
G2474	G2377	G2173	G2173	G2024	G1843	G1692	A1575	A1482	G1205	C1112	C1112	G997	U869	G732
U2477	U2378	A2284	A2176	G2031	C1843	C1693	C1576	C1485	A1206	G1113	G1113	C1000	G872	G734
A2478	G2379	G2285	A2177	G2032	A1844	C1693	C1577	G1486	U1207	G1114	G1114	C1001	U879	G735
C2472	G2380	A2286	G2178	A2032	G1845	U1685	A1580	U1494	U1208	G1115	C1102	C1002	A738	A730
U2473	A2381	A2294	U2179	G2033	A1848	G1695	C1581	G1495	A1216	C1116	A1003	C1003	U739	A740
G2474	U2383	A2303	U2180	G2034	C1848	G1696	C1582	G1507	G1217	U1117	C1004	C1004	G741	G742
U2482	G2384	G2316	A2184	C2043	C1856	G1703	C1583	A1500	U1212	G1129	G1007	G1008	G890	
U2482	U2385	G2317	U2187	G2044	G1863	A1710	U1583	C1501	A1213	G1130	A1011	A1011	G891	G745
A2480	U2386	G2317	G2188	G2045	A1865	G1711	U1584	G1507	G1218	G1135	G1014	A1015	A897	U746
U2490	U2387	C2320	C2189	A2046	C1866	G1712	C1586	A1510	C1219	G1140	C1022	A1025	A898	U747
A2497	U2390	G2328	A2190	G2065	C1871	U1713	U1590	A1518	U1226	U1141	G1030	C1030	G900	U748
G2500	C2391	G2329	C2191	A2066	A1872	A1715	U1591	C1521	C1227	G1142	A1032	A1032	A908	C749
G2503	A2395	U2330	U2195	A2070	U1875	G1717	U1592	G1522	U1228	G1143	A1033	A1033	U915	A756
C2507	A2396	U2331	G2196	G2074	A1876	G1720	U1593	C1522	C1227	U1144	G1043	G1043	U928	U760
A2510	A2399	U2332	G2204	G2075	U1877	G1724	G1605	G1529	G1238	G1162	A1047	A1047	U925	U764
A2511	C2402	U2333	C2206	A2076	G1878	G1724	U1606	G1530	C1239	A1163	A1048	A1048	U926	G765
A2512	U2403	U2334	U2215	G2086	C1892	U1728	G1505	U1529	G1240	A1164	G1049	G1049	C921	G766
U2515	G2404	G2335	G2216	C2087	C1893	U1730	U1597	G1539	U1389	G1165	A1058	A1058	G924	
C2519	G2407	G2336	U2217	C2088	A1894	A1731	U1598	C1531	U1389	G1176	U1060	U1060	U935	U801
G2528	G2408	G2338	C2220	U2091	A1895	G1736	U1599	G1532	G1391	U1178	G1063	G1063	C813	
A2529	U2418	A2340	A2221	U2092	C1900	A1737	G1600	U1533	A1401	U1179	G1063	G1063	U942	G817
A2532	A2421	G2342	C2224	G2093	U1911	G1754	U1605	C1534	A1402	G1180	A1074	A1074	A944	
U2537	U2424	G2343	G2230	G2094	A1916	A1755	G1506	G1538	C1403	G1181	U1075	U1075	U947	G828
A2538	U2425	G2344	C2230	G2095	G1917	G1756	A1616	A1539	G1252	C1182	A1076	A1076	A830	
U2544	G2426	U2345	G2234	G2104	G1946	G1758	C1617	U1540	G1253	U1183	U1076	U1076	U947	A831
G2545	U2427	G2346	G2235	G2105	U1946	A1759	U1620	A1542	G1255	G1180	A1074	A1074	U947	
U2549	G2428	A2351	G2236	A2106	U1947	A1759	U1623	A1543	C1260	G1181	A1074	A1074	U947	
G2549	A2429	C2352	C2243	G2107	C1948	G1769	U1624	A1550	A1415	C1182	A1076	A1076	U947	
	U2430	U2353	A2244	A2109	G1949	G1786	G1625	G1550	A1416	U1183	U1076	U1076	U947	
	C2431	G2354			G1950		G1626	U1627	C1421	U1184	U1077	U1077	G971	
							A1628	G1629						
							U1630							
							A1631							
							G1632							



• Molecule 10: 50S ribosomal protein L2

Chain K: 88% 12%



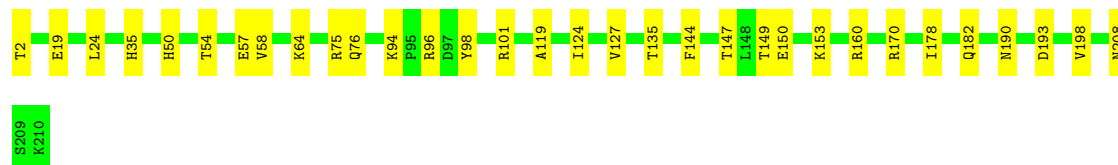
• Molecule 11: 50S ribosomal protein L3

Chain L: 89% 11%



• Molecule 12: 50S ribosomal protein L4

Chain M: 85% 15%



• Molecule 13: 50S ribosomal protein L5

Chain O: 83% 17%

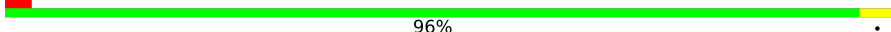


- Molecule 14: 50S ribosomal protein L6

Chain P:  88% 12%



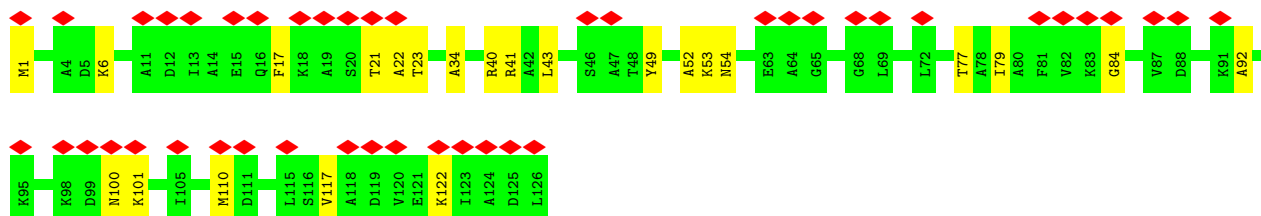
- Molecule 15: 50S ribosomal protein L9

Chain Q:  96%



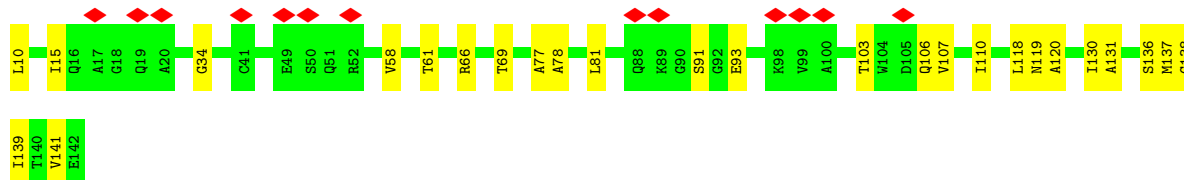
- Molecule 16: 50S ribosomal protein L10

Chain R:  35% 82% 18%



- Molecule 17: 50S ribosomal protein L11

Chain S:  10% 80% 20%



- Molecule 18: 50S ribosomal protein L13

Chain T:  90% 10%



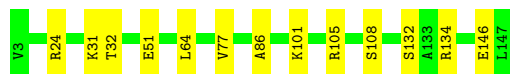
- Molecule 19: 50S ribosomal protein L14

Chain U:  88% 12%



- Molecule 20: 50S ribosomal protein L15

Chain V:  91% 9%



- Molecule 21: 50S ribosomal protein L17

Chain J:  86% 14%



- Molecule 22: 50S ribosomal protein L18

Chain D:  89% 11%

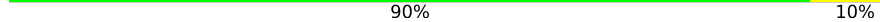


- Molecule 23: 50S ribosomal protein L19

Chain C:  90% 10%



- Molecule 24: 50S ribosomal protein L20

Chain W:  90% 10%



- Molecule 25: 50S ribosomal protein L21

Chain X:  93% 7%



- Molecule 26: 50S ribosomal protein L22

Chain Y:  89% 11%



- Molecule 27: 50S ribosomal protein L23

Chain Z:  93% 7%



- Molecule 28: 50S ribosomal protein L24

Chain 1:  77% 15% 8%



- Molecule 29: 50S ribosomal protein L25

Chain 2:  76% 18% 6%



- Molecule 30: 50S ribosomal protein L27

Chain 4:  94% 6%



- Molecule 31: 50S ribosomal protein L29

Chain 6:  91% 9%



- Molecule 32: 50S ribosomal protein L30

Chain 7:  78% 22%



- Molecule 33: 50S ribosomal protein L32

Chain 8:  91% 9%



- Molecule 34: 50S ribosomal protein L34

Chain 0:  87% 13%



- Molecule 35: 50S ribosomal protein L35

Chain x:  87% 13%



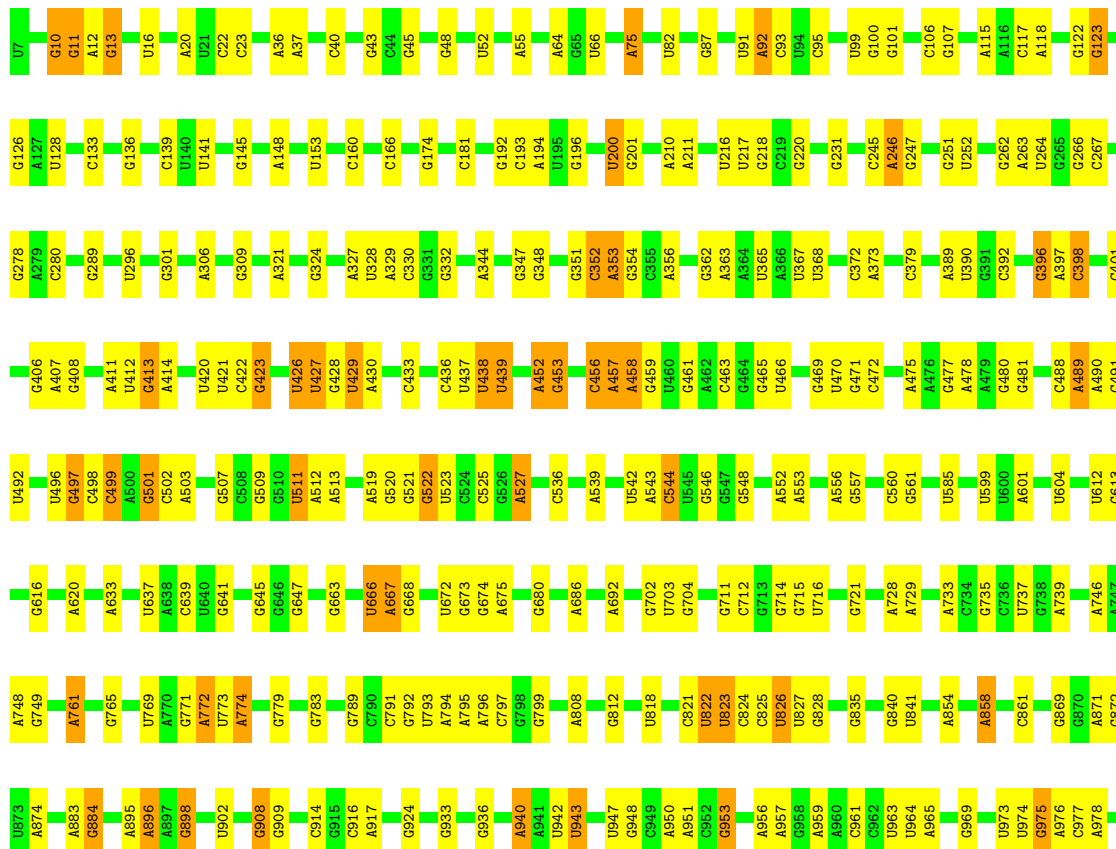
- Molecule 36: 50S ribosomal protein L36

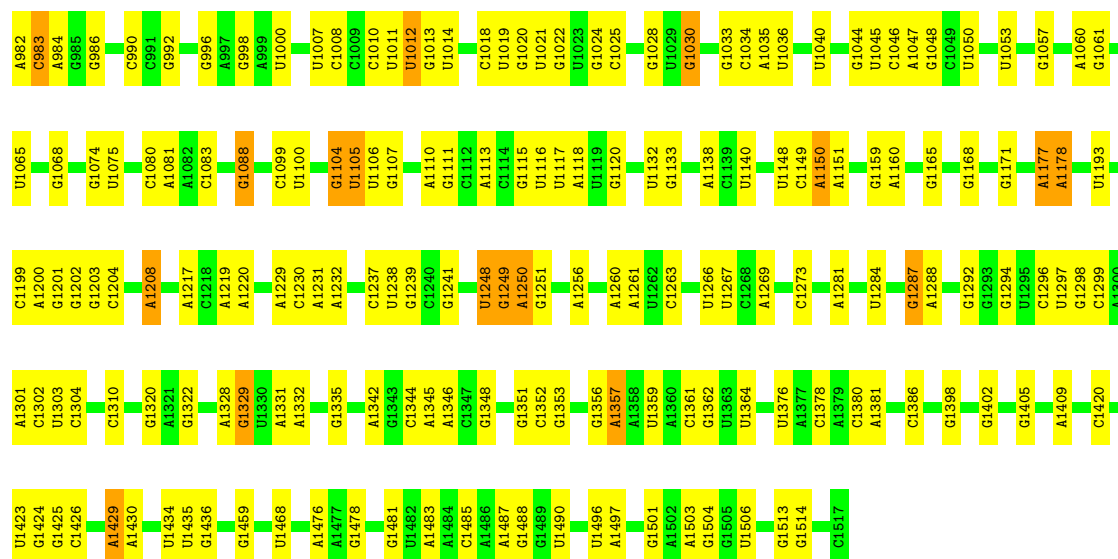
Chain F:  78% 22%



- Molecule 37: 16S rRNA (1511-MER)

Chain a:  68% 28% .





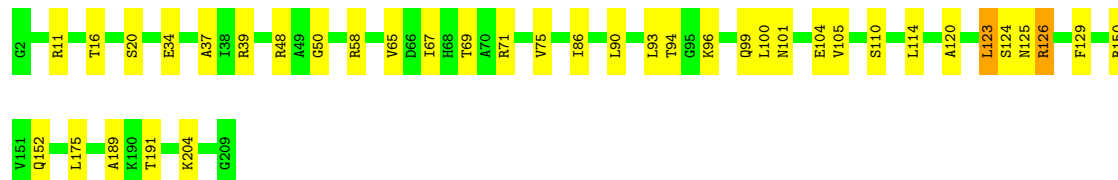
• Molecule 38: 30S ribosomal protein S22

Chain b: 88% 12%



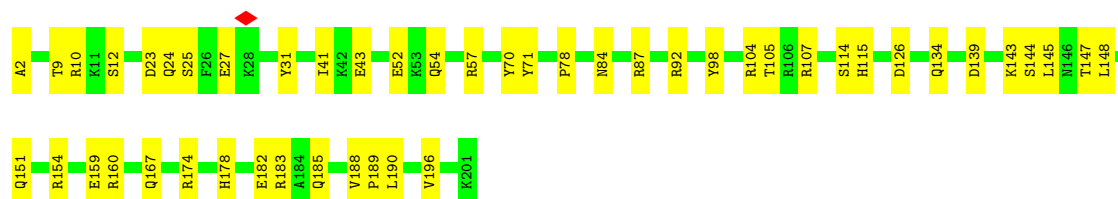
• Molecule 39: 30S ribosomal protein S3

Chain G: 82% 17%



• Molecule 40: 30S ribosomal protein S4

Chain e: 76% 24%



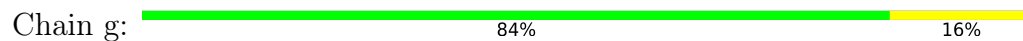
• Molecule 41: 30S ribosomal protein S5

Chain f: 89% 11%

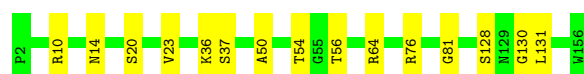
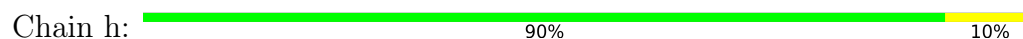




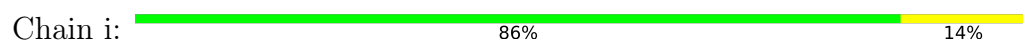
- Molecule 42: 30S ribosomal protein S6



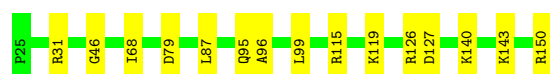
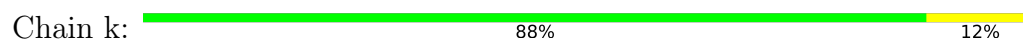
- Molecule 43: 30S ribosomal protein S7



- Molecule 44: 30S ribosomal protein S8



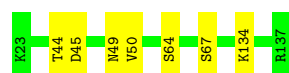
- Molecule 45: 30S ribosomal protein S9



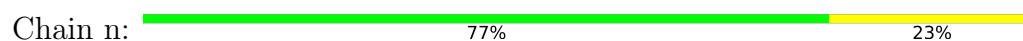
- Molecule 46: 30S ribosomal protein S10



- Molecule 47: 30S ribosomal protein S11

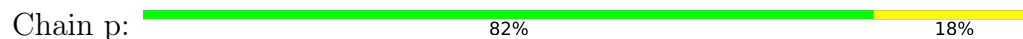


- Molecule 48: 30S ribosomal protein S12

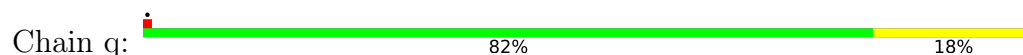




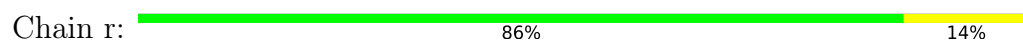
- Molecule 49: 30S ribosomal protein S15



- Molecule 50: 30S ribosomal protein S16



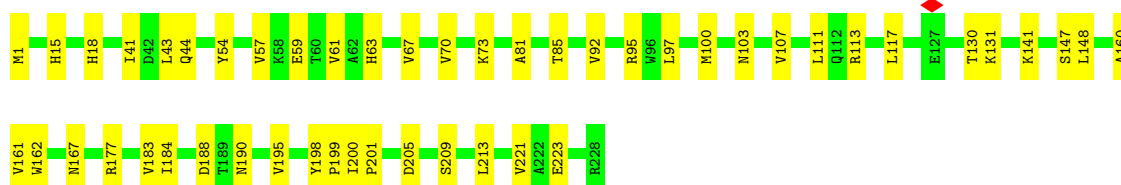
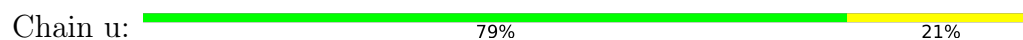
- Molecule 51: 30S ribosomal protein S17



- Molecule 52: 30S ribosomal protein S20



- Molecule 53: 30S ribosomal protein S2



- Molecule 54: mRNA





● Molecule 58: 30S ribosomal protein S14



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	36321	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 ($e^-/\text{\AA}^2$)	66.59	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.041	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.003	Depositor
Map size ($\text{\AA}$)	423.72, 423.72, 423.72	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.84744, 0.84744, 0.84744	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	c	0.65	0/430	1.08	6/577 (1.0%)
2	y	0.75	2/616 (0.3%)	1.02	10/825 (1.2%)
3	E	0.32	0/1833	0.46	0/2854
4	d	0.87	4/680 (0.6%)	1.27	14/915 (1.5%)
5	B	0.49	0/2821	0.46	0/4396
6	j	0.45	0/942	0.59	0/1260
7	N	0.66	0/1118	0.49	0/1506
8	3	0.74	0/191	0.47	0/247
9	A	0.57	0/75001	0.44	0/117027
10	K	0.72	0/2153	0.50	0/2895
11	L	0.69	0/1609	0.50	0/2165
12	M	0.66	0/1592	0.46	0/2153
13	O	0.49	0/1467	0.46	0/1973
14	P	0.39	0/1369	0.41	0/1848
15	Q	0.27	0/1027	0.44	0/1398
16	R	0.23	0/925	0.47	0/1246
17	S	0.22	0/1006	0.49	0/1364
18	T	0.65	0/1157	0.45	0/1567
19	U	0.66	0/946	0.44	0/1268
20	V	0.65	0/1091	0.45	0/1457
21	J	0.69	0/945	0.47	0/1267
22	D	0.54	0/966	0.46	0/1298
23	C	0.62	0/921	0.48	0/1236
24	W	0.73	0/1000	0.47	0/1341
25	X	0.66	0/764	0.43	0/1030
26	Y	0.70	0/887	0.47	0/1204
27	Z	0.60	0/766	0.43	0/1030
28	1	0.52	0/738	0.39	0/987
29	2	0.40	0/1361	0.42	0/1858
30	4	0.72	0/595	0.41	0/798
31	6	0.56	0/534	0.39	0/713
32	7	0.66	0/477	0.45	0/640
33	8	0.73	0/427	0.51	0/572
34	0	0.75	0/380	0.51	0/500

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	x	0.75	0/507	0.41	0/672
36	F	0.64	0/303	0.46	0/401
37	a	0.50	0/36309	0.42	0/56657
38	b	0.61	0/280	0.52	0/359
39	G	0.44	0/1684	0.52	1/2261 (0.0%)
40	e	0.41	0/1672	0.48	0/2251
41	f	0.52	0/1312	0.44	0/1772
42	g	0.51	0/782	0.48	0/1059
43	h	0.43	0/1252	0.45	0/1690
44	i	0.57	0/1025	0.42	0/1385
45	k	0.46	0/1012	0.48	0/1362
46	l	0.41	0/802	0.43	0/1086
47	m	0.51	0/873	0.45	0/1180
48	n	0.55	0/969	0.47	0/1294
49	p	0.57	0/729	0.43	0/977
50	q	0.53	0/908	0.52	0/1226
51	r	0.49	0/759	0.46	0/1016
52	t	0.53	0/663	0.42	0/882
53	u	0.29	0/1822	0.45	0/2457
54	v	0.26	0/436	0.37	0/679
55	I	0.28	0/1144	0.56	0/1560
56	H	0.33	0/613	0.46	0/835
57	o	0.49	0/549	0.50	0/737
58	9	0.46	0/830	0.43	0/1106
All	All	0.55	6/165970 (0.0%)	0.46	31/248319 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	y	24	THR	C-N	8.57	1.44	1.33
4	d	51	VAL	N-CA	-7.31	1.38	1.46
4	d	71	LEU	C-N	6.59	1.42	1.33
4	d	15	LEU	C-N	5.65	1.41	1.33
4	d	71	LEU	N-CA	-5.18	1.39	1.46
2	y	14	GLY	C-N	5.06	1.40	1.33

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	51	VAL	N-CA-C	11.56	122.25	110.23
4	d	37	ARG	N-CA-C	9.17	130.32	110.80
4	d	37	ARG	CA-C-N	8.44	133.81	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	37	ARG	C-N-CA	8.44	133.81	122.84
1	c	23	THR	O-C-N	-7.52	113.46	123.23
4	d	58	VAL	CA-C-N	-7.45	111.95	119.92
4	d	58	VAL	C-N-CA	-7.45	111.95	119.92
2	y	24	THR	N-CA-C	-7.36	100.16	110.31
4	d	34	TRP	N-CA-C	6.93	118.62	111.14
4	d	37	ARG	CB-CA-C	-6.57	97.34	110.42
2	y	25	PRO	O-C-N	-6.44	115.14	123.00
4	d	12	ASP	N-CA-C	-6.27	101.14	110.23
2	y	17	VAL	CA-C-N	6.22	134.08	123.01
2	y	17	VAL	C-N-CA	6.22	134.08	123.01
2	y	26	ARG	CA-C-N	5.71	131.62	121.75
2	y	26	ARG	C-N-CA	5.71	131.62	121.75
4	d	36	ARG	N-CA-C	-5.68	98.71	110.80
4	d	11	VAL	O-C-N	-5.64	117.11	123.20
1	c	52	GLU	CA-C-N	5.53	131.66	121.70
1	c	52	GLU	C-N-CA	5.53	131.66	121.70
1	c	10	LYS	N-CA-C	5.44	117.21	111.28
4	d	12	ASP	CA-C-N	5.35	127.99	120.28
4	d	12	ASP	C-N-CA	5.35	127.99	120.28
2	y	14	GLY	CA-C-N	5.24	130.04	122.44
2	y	14	GLY	C-N-CA	5.24	130.04	122.44
1	c	26	ASN	CA-C-N	5.17	128.05	120.71
1	c	26	ASN	C-N-CA	5.17	128.05	120.71
2	y	29	ASP	CA-C-N	5.15	125.13	120.03
2	y	29	ASP	C-N-CA	5.15	125.13	120.03
39	G	125	ASN	N-CA-C	5.13	116.88	111.28
4	d	70	LYS	O-C-N	-5.08	116.69	122.93

There are no chirality outliers.

There are no planarity outliers.

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	c	423	0	442	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	y	605	0	618	24	0
3	E	1642	0	834	49	0
4	d	662	0	677	84	0
5	B	2522	0	1285	22	0
6	j	935	0	986	19	0
7	N	1092	0	1128	12	0
8	3	189	0	205	2	0
9	A	66981	0	33700	363	0
10	K	2110	0	2165	23	0
11	L	1587	0	1630	22	0
12	M	1569	0	1607	22	0
13	O	1445	0	1476	26	0
14	P	1348	0	1399	17	0
15	Q	1018	0	988	5	0
16	R	918	0	959	21	0
17	S	990	0	1021	19	0
18	T	1130	0	1167	10	0
19	U	938	0	1000	12	0
20	V	1078	0	1151	11	0
21	J	928	0	972	12	0
22	D	956	0	991	10	0
23	C	907	0	938	8	0
24	W	988	0	1038	12	0
25	X	754	0	802	5	0
26	Y	873	0	909	9	0
27	Z	756	0	802	6	0
28	1	732	0	782	12	0
29	2	1347	0	1373	20	0
30	4	586	0	601	4	0
31	6	531	0	541	6	0
32	7	474	0	500	12	0
33	8	423	0	463	4	0
34	0	377	0	411	5	0
35	x	502	0	541	8	0
36	F	299	0	324	5	0
37	a	32439	0	16321	201	0
38	b	280	0	342	4	0
39	G	1660	0	1707	32	0
40	e	1641	0	1668	37	0
41	f	1296	0	1360	17	0
42	g	771	0	797	9	0
43	h	1232	0	1282	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	i	1010	0	1046	15	0
45	k	994	0	1050	12	0
46	l	788	0	819	21	0
47	m	855	0	863	6	0
48	n	958	0	1045	24	0
49	p	720	0	760	12	0
50	q	891	0	935	16	0
51	r	748	0	795	12	0
52	t	660	0	712	6	0
53	u	1793	0	1839	33	0
54	v	388	0	196	2	0
55	I	1126	0	1122	52	0
56	H	593	0	569	17	0
57	o	543	0	582	9	0
58	9	819	0	866	24	0
All	All	152820	0	103102	1207	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 5.

All (1207) 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)
3:E:503:C:C5	3:E:572:U:C4	1.95	1.52
3:E:503:C:C6	3:E:572:U:C4	2.04	1.44
3:E:503:C:C6	3:E:572:U:C5	2.09	1.41
55:I:668:THR:HG22	55:I:718:PHE:CD1	1.71	1.25
3:E:503:C:C5	3:E:572:U:C5	2.24	1.21
1:c:11:LEU:HD11	1:c:26:ASN:N	1.55	1.20
1:c:11:LEU:CD1	1:c:26:ASN:HB3	1.80	1.12
4:d:45:ILE:O	4:d:62:VAL:O	1.67	1.11
1:c:11:LEU:HD11	1:c:26:ASN:CB	1.82	1.10
55:I:668:THR:HG22	55:I:718:PHE:CE1	1.87	1.09
1:c:11:LEU:HD11	1:c:26:ASN:HB3	1.32	1.09
4:d:44:PHE:O	4:d:62:VAL:HG11	1.52	1.09
3:E:503:C:C6	3:E:572:U:O4	2.04	1.08
4:d:55:ARG:HD2	37:a:940:A:N7	1.75	1.02
2:y:1:SER:H3	2:y:29:ASP:HB3	1.22	1.01
1:c:11:LEU:HD11	1:c:26:ASN:CA	1.92	0.98
3:E:503:C:H6	3:E:572:U:O4	1.41	0.97
4:d:46:GLY:O	4:d:61:PHE:CE1	2.17	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:11:LEU:CD1	1:c:26:ASN:N	2.28	0.95
4:d:44:PHE:CE2	4:d:49:PHE:CZ	2.55	0.94
4:d:44:PHE:O	4:d:62:VAL:CG1	2.15	0.94
3:E:503:C:H5	3:E:572:U:C4	1.79	0.94
4:d:57:HIS:HB3	55:I:660:LEU:HB2	1.50	0.94
4:d:28:LYS:NZ	4:d:47:HIS:HE1	1.67	0.92
10:K:155:LEU:HD13	10:K:177:MET:HE1	1.52	0.91
55:I:668:THR:CG2	55:I:718:PHE:CD1	2.53	0.90
4:d:55:ARG:HD2	37:a:940:A:C5	2.06	0.90
45:k:68:ILE:HD12	45:k:99:LEU:HD23	1.55	0.88
55:I:668:THR:HG22	55:I:718:PHE:HD1	1.36	0.88
4:d:46:GLY:HA2	4:d:61:PHE:CE1	2.09	0.87
39:G:123:LEU:HD11	39:G:129:PHE:HA	1.55	0.87
2:y:1:SER:N	2:y:29:ASP:HB3	1.90	0.86
4:d:44:PHE:CD2	4:d:49:PHE:CZ	2.63	0.86
4:d:44:PHE:CE2	4:d:49:PHE:CE2	2.64	0.86
4:d:46:GLY:O	4:d:61:PHE:HE1	1.54	0.86
4:d:28:LYS:HD3	4:d:47:HIS:ND1	1.92	0.84
37:a:91:U:O2'	37:a:92:A:O5'	1.96	0.84
37:a:363:A:OP2	48:n:31:ARG:NH1	2.12	0.82
37:a:1497:A:OP2	38:b:18:ARG:NH2	2.12	0.82
3:E:503:C:C5	3:E:572:U:N3	2.48	0.82
1:c:11:LEU:CD1	1:c:26:ASN:CB	2.50	0.81
4:d:52:HIS:O	4:d:56:LYS:O	1.99	0.81
9:A:1204:A:O2'	9:A:1205:G:N7	2.12	0.81
9:A:2379:G:O2'	9:A:2380:G:O4'	1.99	0.80
39:G:123:LEU:HD21	39:G:129:PHE:HB3	1.64	0.80
3:E:503:C:C6	3:E:572:U:H5	1.99	0.80
48:n:50:ARG:NH1	48:n:89:ASP:OD2	2.14	0.80
5:B:80:C:H42	5:B:96:A:H61	1.30	0.79
37:a:956:A:OP1	58:9:69:ARG:NH2	2.15	0.79
40:e:25:SER:OG	40:e:31:TYR:OH	1.99	0.79
9:A:2357:A:N7	9:A:2380:G:C2	2.50	0.79
55:I:668:THR:CG2	55:I:718:PHE:HD1	1.92	0.79
37:a:503:A:OP1	48:n:116:ARG:NH2	2.16	0.79
9:A:80:G:OP1	28:1:94:LYS:NZ	2.16	0.78
37:a:489:A:N7	37:a:523:U:O2'	2.15	0.78
37:a:23:C:OP1	41:f:155:SER:OG	2.01	0.78
37:a:438:U:O2'	37:a:439:U:O2	2.02	0.77
9:A:1379:G:OP1	33:8:16:ARG:NH2	2.17	0.77
9:A:1189:G:N2	9:A:1219:U:O4	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:32:C:O2	5:B:54:A:N6	2.18	0.77
9:A:1626:G:O2'	9:A:1627:U:O4'	2.03	0.77
39:G:48:ARG:O	39:G:71:ARG:NH2	2.18	0.77
4:d:28:LYS:HZ3	4:d:47:HIS:HE1	1.32	0.77
9:A:1305:G:OP1	20:V:32:THR:OG1	2.03	0.76
9:A:2750:G:OP2	14:P:154:ARG:NH2	2.18	0.76
37:a:309:G:OP1	50:q:28:ARG:NH2	2.18	0.76
9:A:2244:A:O2'	9:A:2246:U:OP2	2.02	0.76
9:A:3014:A:O2'	9:A:3015:C:O5'	2.04	0.75
37:a:1099:C:OP2	45:k:31:ARG:NH2	2.19	0.75
4:d:44:PHE:CD2	4:d:49:PHE:CE2	2.75	0.75
4:d:44:PHE:CD2	4:d:49:PHE:HZ	2.01	0.75
9:A:830:A:OP2	49:p:89:ARG:NH1	2.19	0.75
9:A:993:G:O2'	9:A:994:A:O4'	2.02	0.75
9:A:2184:A:O2'	37:a:1468:U:O2'	2.04	0.75
37:a:356:A:N3	37:a:368:U:O2'	2.19	0.75
4:d:45:ILE:HG23	4:d:63:THR:C	2.12	0.75
9:A:210:G:OP1	34:0:28:ARG:NH2	2.20	0.75
13:O:117:ARG:NH1	13:O:143:SER:O	2.19	0.75
37:a:772:A:O2'	37:a:774:A:N7	2.18	0.75
37:a:527:A:OP2	40:e:2:ALA:N	2.20	0.75
4:d:28:LYS:NZ	4:d:47:HIS:CE1	2.54	0.74
13:O:141:GLU:OE1	13:O:143:SER:N	2.20	0.74
37:a:1202:G:O2'	37:a:1203:G:H5'	1.87	0.74
9:A:1205:G:O2'	9:A:1208:U:OP1	2.05	0.74
53:u:54:TYR:OH	53:u:223:GLU:OE1	2.04	0.74
9:A:891:G:N7	9:A:908:A:O2'	2.19	0.74
9:A:1202:A:N3	9:A:1223:U:O2'	2.17	0.74
9:A:2870:C:OP2	9:A:2956:G:O2'	2.06	0.74
19:U:120:GLU:OE1	23:C:64:SER:OG	2.05	0.74
9:A:605:G:OP2	33:8:14:ARG:NH2	2.21	0.74
9:A:1112:C:OP1	24:W:53:ARG:NH2	2.21	0.74
9:A:2587:U:OP2	35:x:43:ARG:NH2	2.20	0.74
9:A:1186:G:N2	9:A:1213:A:O2'	2.21	0.73
4:d:14:HIS:NE2	37:a:998:G:OP1	2.21	0.73
5:B:5:C:OP1	5:B:62:C:O2'	2.06	0.73
9:A:1532:G:O2'	9:A:1803:A:N1	2.16	0.73
9:A:1564:A:O2'	9:A:1565:A:O4'	2.06	0.73
9:A:1886:A:O2'	9:A:1892:G:N7	2.18	0.73
37:a:525:C:OP2	40:e:57:ARG:NH1	2.22	0.73
9:A:885:G:OP1	34:0:11:ASN:ND2	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:858:A:O2'	9:A:1877:U:OP1	2.07	0.73
9:A:885:G:OP2	34:0:14:ARG:NH2	2.22	0.73
9:A:2900:C:OP1	19:U:31:ARG:NH2	2.21	0.73
41:f:182:ARG:O	44:i:65:LYS:NZ	2.22	0.73
3:E:504:G:N2	3:E:570:G:N1	2.36	0.73
13:O:66:LEU:O	56:H:28:THR:OG1	2.05	0.73
4:d:45:ILE:C	4:d:62:VAL:HG13	2.13	0.72
17:S:61:THR:OG1	17:S:69:THR:O	2.07	0.72
55:I:746:ASN:O	55:I:765:THR:OG1	2.07	0.72
1:c:27:ARG:NH2	9:A:2510:A:OP1	2.22	0.72
9:A:706:G:O2'	12:M:160:ARG:NH2	2.23	0.72
9:A:2557:A:OP1	30:4:75:ARG:NH2	2.22	0.72
40:e:134:GLN:NE2	40:e:178:HIS:O	2.22	0.72
7:N:110:ASP:OD1	7:N:113:THR:OG1	2.06	0.72
9:A:285:U:O2'	9:A:287:A:OP1	2.06	0.72
9:A:1181:G:O2'	17:S:91:SER:O	2.08	0.72
22:D:118:ASP:OD1	22:D:121:ARG:NH1	2.23	0.72
9:A:2176:A:N3	9:A:2784:C:O2'	2.23	0.71
4:d:28:LYS:HG2	4:d:47:HIS:CE1	2.25	0.71
9:A:2669:G:OP1	12:M:75:ARG:NH1	2.23	0.71
37:a:961:C:O2	58:9:59:ARG:NE	2.24	0.71
9:A:2204:G:O2'	9:A:2206:C:OP2	2.07	0.71
37:a:263:A:OP1	52:t:74:ASN:ND2	2.23	0.71
3:E:507:G:OP2	3:E:548:C:N4	2.22	0.71
4:d:78:ARG:NH2	37:a:1303:U:O2'	2.24	0.71
9:A:1500:A:O2'	9:A:1511:U:O2	2.08	0.71
46:l:6:ILE:HD11	46:l:76:ILE:HD11	1.73	0.71
3:E:554:U:O4	3:E:558:A:N6	2.24	0.71
9:A:1696:G:O2'	9:A:1736:G:O6	2.06	0.71
53:u:177:ARG:NH2	53:u:195:VAL:O	2.24	0.71
9:A:2474:G:O2'	9:A:2720:C:OP1	2.06	0.71
37:a:502:C:OP2	48:n:66:TYR:OH	2.04	0.71
3:E:549:G:O6	3:E:565:U:O2	2.09	0.71
9:A:3102:U:O2	21:J:45:ARG:NH2	2.24	0.71
6:j:86:CYS:SG	6:j:87:TYR:N	2.63	0.70
9:A:2727:A:O2'	9:A:2729:G:OP2	2.09	0.70
37:a:246:A:N1	37:a:278:G:O2'	2.21	0.70
4:d:46:GLY:HA2	4:d:61:PHE:CZ	2.26	0.70
39:G:11:ARG:O	39:G:16:THR:OG1	2.08	0.70
9:A:616:A:OP2	18:T:116:ARG:NH2	2.24	0.70
4:d:45:ILE:O	4:d:62:VAL:HG13	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:a:181:C:OP1	37:a:200:U:O2'	2.08	0.70
1:c:17:THR:O	1:c:44:ARG:NH1	2.25	0.70
9:A:2356:G:O2'	9:A:2357:A:O5'	2.08	0.70
12:M:153:LYS:NZ	12:M:190:ASN:OD1	2.23	0.70
51:r:41:GLU:OE2	51:r:43:ARG:NH2	2.25	0.70
16:R:117:VAL:O	16:R:122:LYS:NZ	2.24	0.70
37:a:390:U:O3'	50:q:29:ARG:NH2	2.24	0.70
9:A:2220:C:OP1	19:U:31:ARG:NH1	2.25	0.70
37:a:943:U:OP2	37:a:1204:C:O2'	2.08	0.70
58:9:52:PRO:O	58:9:55:SER:OG	2.05	0.70
37:a:1342:A:OP2	58:9:75:ARG:NH2	2.25	0.70
37:a:133:C:O2'	50:q:65:GLN:OE1	2.09	0.70
1:c:11:LEU:CD1	1:c:25:LYS:C	2.63	0.69
29:2:11:LEU:HD12	29:2:67:LEU:HD12	1.74	0.69
4:d:55:ARG:NH1	37:a:940:A:OP1	2.19	0.69
37:a:1160:A:OP2	45:k:115:ARG:NH2	2.25	0.69
40:e:84:ASN:OD1	40:e:87:ARG:NH2	2.24	0.69
46:l:63:GLU:OE1	58:9:85:ARG:NH1	2.25	0.69
43:h:14:ASN:OD1	43:h:20:SER:N	2.26	0.69
37:a:123:G:O2'	51:r:21:LYS:NZ	2.24	0.69
37:a:396:G:O2'	37:a:398:C:OP1	2.09	0.69
48:n:79:MET:N	48:n:103:ASP:OD2	2.26	0.69
9:A:1189:G:N2	9:A:1208:U:O4	2.18	0.69
37:a:965:A:OP1	58:9:6:LYS:NZ	2.25	0.69
37:a:998:G:O2'	37:a:1199:C:O2'	2.08	0.69
48:n:27:SER:OG	48:n:29:GLN:O	2.08	0.69
4:d:28:LYS:HD3	4:d:47:HIS:CE1	2.27	0.69
5:B:42:C:N4	13:O:74:VAL:O	2.24	0.69
7:N:77:LYS:NZ	7:N:84:GLY:O	2.25	0.69
9:A:81:A:OP1	28:1:4:HIS:NE2	2.26	0.69
9:A:879:A:OP1	10:K:208:LYS:NZ	2.26	0.69
37:a:439:U:O4	37:a:478:A:N6	2.20	0.69
46:l:46:LYS:NZ	46:l:66:GLU:OE1	2.25	0.69
37:a:525:C:OP2	40:e:54:GLN:NE2	2.26	0.69
9:A:1008:G:O2'	55:I:696:GLU:OE2	2.10	0.69
9:A:2257:A:O2'	9:A:2259:G:OP2	2.11	0.69
9:A:255:A:O2'	9:A:472:C:OP2	2.11	0.68
9:A:861:U:O4	11:L:142:GLN:NE2	2.27	0.68
9:A:2881:A:O3'	14:P:161:LYS:NZ	2.26	0.68
37:a:1148:U:OP1	37:a:1150:A:N6	2.26	0.68
9:A:2883:G:OP2	14:P:159:LYS:NZ	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:32:LYS:HZ2	4:d:53:ASP:CG	2.02	0.68
9:A:316:U:O2'	9:A:317:G:OP1	2.10	0.68
9:A:1381:G:O2'	9:A:2236:G:O6	2.09	0.68
9:A:2357:A:N7	9:A:2380:G:N2	2.41	0.68
37:a:748:A:N3	37:a:1496:U:O2'	2.24	0.68
37:a:413:G:N7	40:e:24:GLN:NE2	2.42	0.68
46:l:24:LYS:HD3	46:l:90:ILE:HD11	1.76	0.68
9:A:974:G:O2'	9:A:1031:G:O6	2.10	0.68
9:A:1359:G:O2'	12:M:35:HIS:NE2	2.25	0.68
37:a:122:G:OP1	37:a:585:U:O2'	2.05	0.68
57:o:24:LEU:HD13	57:o:32:ILE:HD11	1.75	0.68
37:a:799:G:O6	38:b:2:GLY:N	2.26	0.68
9:A:49:A:OP2	9:A:114:G:N1	2.26	0.68
50:q:8:THR:HG22	50:q:29:ARG:O	1.93	0.68
9:A:1105:C:O2'	9:A:1118:A:N3	2.23	0.68
9:A:2795:C:O2'	11:L:157:PRO:HD3	1.93	0.68
9:A:3012:U:O2'	9:A:3030:A:N3	2.25	0.68
9:A:3013:C:O2'	9:A:3113:A:N6	2.27	0.68
42:g:92:ARG:NH2	42:g:94:ASP:OD2	2.26	0.68
9:A:163:U:OP2	15:Q:121:LYS:NZ	2.21	0.68
47:m:45:ASP:OD2	47:m:49:ASN:N	2.27	0.68
55:I:753:THR:O	55:I:756:ASN:ND2	2.27	0.68
53:u:73:LYS:NZ	53:u:205:ASP:OD1	2.21	0.67
9:A:1514:C:OP1	27:Z:85:LYS:NZ	2.23	0.67
9:A:227:A:N1	9:A:505:C:O2'	2.27	0.67
4:d:56:LYS:HG2	55:I:660:LEU:HD13	1.77	0.67
9:A:368:U:O2	9:A:434:G:O6	2.13	0.67
9:A:1605:G:N2	9:A:1606:G:O6	2.27	0.67
7:N:106:LEU:HD22	7:N:118:LEU:HD21	1.77	0.67
12:M:64:LYS:NZ	12:M:76:GLN:O	2.28	0.67
29:2:122:THR:OG1	29:2:182:VAL:O	2.06	0.67
2:y:6:VAL:HG23	2:y:7:THR:HG23	1.77	0.67
9:A:183:G:O2'	9:A:216:A:N3	2.27	0.67
9:A:2043:C:O2'	9:A:2195:U:OP2	2.12	0.67
37:a:457:A:O2'	37:a:458:A:O5'	2.13	0.67
37:a:715:G:O2'	57:o:72:ASN:OD1	2.13	0.67
55:I:670:VAL:HG11	55:I:717:VAL:HA	1.75	0.67
9:A:2674:A:OP1	9:A:2721:A:O2'	2.11	0.66
1:c:11:LEU:HD12	1:c:25:LYS:C	2.20	0.66
3:E:565:U:O3'	3:E:567:C:N4	2.29	0.66
55:I:680:THR:N	55:I:684:GLY:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1163:A:OP1	9:A:1164:A:O2'	2.14	0.66
9:A:1675:U:O2'	9:A:1676:G:N7	2.28	0.66
37:a:1199:C:H2'	37:a:1200:A:H8	1.60	0.66
51:r:60:LYS:NZ	51:r:85:THR:OG1	2.26	0.66
9:A:2490:A:N6	9:A:2497:A:OP2	2.27	0.66
37:a:1376:U:HO2'	37:a:1485:C:HO2'	1.37	0.66
1:c:11:LEU:HD13	1:c:26:ASN:HB3	1.75	0.66
4:d:45:ILE:CG2	4:d:63:THR:HA	2.26	0.66
9:A:30:U:O4	9:A:534:G:O2'	2.10	0.66
37:a:363:A:OP1	48:n:58:THR:OG1	2.13	0.66
49:p:29:VAL:O	49:p:33:THR:OG1	2.10	0.66
6:j:102:ARG:NH1	37:a:933:G:OP2	2.29	0.66
4:d:32:LYS:HB2	55:I:656:ALA:HB3	1.77	0.66
9:A:1825:C:N4	9:A:1840:G:OP2	2.23	0.66
9:A:2648:C:O2	9:A:2653:G:O2'	2.12	0.66
16:R:40:ARG:NH1	16:R:49:TYR:O	2.28	0.66
37:a:1104:G:N2	37:a:1105:U:O4	2.29	0.66
53:u:59:GLU:O	53:u:63:HIS:ND1	2.26	0.66
9:A:239:U:OP1	9:A:684:G:N2	2.29	0.65
37:a:1361:C:N3	43:h:76:ARG:NH2	2.44	0.65
4:d:55:ARG:HB3	37:a:940:A:C6	2.31	0.65
9:A:499:G:OP2	9:A:2630:A:O2'	2.09	0.65
9:A:3086:U:OP2	9:A:3087:G:O2'	2.14	0.65
9:A:830:A:OP1	49:p:64:ARG:NH1	2.30	0.65
9:A:1129:G:OP2	24:W:66:ASN:ND2	2.29	0.65
9:A:1411:G:OP1	9:A:2933:G:O2'	2.13	0.65
9:A:1441:C:O2'	9:A:2234:G:O2'	2.13	0.65
37:a:673:G:O2'	43:h:81:GLY:O	2.14	0.65
5:B:14:A:O2'	5:B:71:C:O2'	2.02	0.65
7:N:67:ASN:O	7:N:101:ARG:NH2	2.30	0.65
9:A:80:G:N2	9:A:100:A:OP2	2.30	0.65
9:A:1188:A:N6	9:A:1214:A:O2'	2.30	0.65
37:a:1357:A:OP1	43:h:36:LYS:NZ	2.22	0.65
12:M:149:THR:OG1	12:M:193:ASP:OD2	2.12	0.65
55:I:675:ILE:HD11	55:I:710:TRP:CB	2.27	0.65
26:Y:75:THR:OG1	26:Y:116:SER:OG	2.15	0.64
3:E:503:C:N1	3:E:572:U:C5	2.63	0.64
4:d:45:ILE:HG23	4:d:63:THR:HA	1.80	0.64
9:A:286:G:N2	9:A:287:A:N7	2.46	0.64
9:A:2482:U:O2'	9:A:2651:C:OP2	2.15	0.64
37:a:1332:A:OP1	45:k:143:LYS:NZ	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:4:SER:OG	37:a:1296:C:OP2	2.10	0.64
27:Z:50:PHE:O	27:Z:91:LYS:NZ	2.30	0.64
37:a:456:C:O2'	37:a:457:A:N7	2.23	0.64
3:E:503:C:OP2	3:E:572:U:O4	2.15	0.64
4:d:27:THR:OG1	4:d:29:GLN:OE1	2.09	0.64
4:d:28:LYS:CD	4:d:47:HIS:CE1	2.80	0.64
4:d:46:GLY:O	4:d:61:PHE:CD1	2.50	0.64
4:d:45:ILE:HG23	4:d:63:THR:CA	2.26	0.64
9:A:1111:G:OP2	24:W:51:ARG:NH2	2.30	0.64
9:A:2391:G:O2'	9:A:2392:A:O4'	2.10	0.64
42:g:24:GLU:OE1	42:g:31:ARG:NH2	2.30	0.64
56:H:16:ASP:OD2	56:H:57:SER:OG	2.15	0.64
9:A:1754:G:N2	9:A:1759:A:N1	2.46	0.64
40:e:151:GLN:OE1	40:e:154:ARG:NH1	2.30	0.64
21:J:51:LEU:HD13	21:J:70:ILE:HD11	1.80	0.64
37:a:106:C:O2'	50:q:26:ARG:O	2.16	0.64
37:a:965:A:O2'	37:a:1030:G:OP2	2.13	0.64
37:a:858:A:H1'	44:i:12:THR:HG21	1.79	0.64
9:A:3014:A:N6	9:A:3113:A:OP2	2.29	0.64
13:O:19:ILE:HD12	13:O:179:ALA:HB1	1.79	0.64
32:7:38:GLU:N	32:7:38:GLU:OE1	2.30	0.64
56:H:16:ASP:OD2	56:H:54:THR:OG1	2.10	0.64
9:A:2691:C:OP1	36:F:6:SER:OG	2.10	0.63
9:A:2796:A:OP2	11:L:156:THR:HB	1.97	0.63
4:d:32:LYS:HG3	4:d:34:TRP:CZ3	2.33	0.63
9:A:414:A:O2'	9:A:416:C:OP2	2.14	0.63
12:M:127:VAL:O	12:M:198:VAL:HG23	1.99	0.63
40:e:167:GLN:N	40:e:167:GLN:OE1	2.32	0.63
9:A:993:G:N2	9:A:1015:A:OP2	2.31	0.63
37:a:436:C:H4'	40:e:148:LEU:HD23	1.81	0.63
9:A:1649:C:O2'	9:A:1789:A:OP2	2.13	0.63
13:O:24:GLN:OE1	13:O:29:TYR:N	2.32	0.63
37:a:716:U:O2'	42:g:90:VAL:O	2.14	0.63
9:A:745:G:OP1	35:x:19:THR:OG1	2.15	0.63
2:y:39:LEU:O	2:y:42:GLU:N	2.32	0.63
9:A:2519:C:OP2	22:D:24:ARG:NH2	2.31	0.62
23:C:33:GLU:OE1	23:C:36:LYS:NZ	2.32	0.62
9:A:735:U:O2'	9:A:2574:C:OP1	2.17	0.62
37:a:437:U:O2'	40:e:115:HIS:ND1	2.24	0.62
39:G:11:ARG:NH2	39:G:175:LEU:O	2.32	0.62
39:G:123:LEU:HD21	39:G:129:PHE:CB	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:287:A:N1	9:A:299:G:N2	2.46	0.62
9:A:1200:U:O2	16:R:40:ARG:NH2	2.32	0.62
9:A:1573:U:O2'	9:A:1597:G:N1	2.32	0.62
4:d:6:LYS:NZ	37:a:1296:C:OP1	2.29	0.62
39:G:123:LEU:HD21	39:G:129:PHE:CA	2.29	0.62
2:y:4:CYS:SG	2:y:5:GLN:N	2.73	0.62
4:d:57:HIS:HB3	55:I:660:LEU:CB	2.28	0.62
12:M:24:LEU:HD21	12:M:208:ASN:HB2	1.81	0.62
56:H:34:THR:HG21	56:H:47:PRO:CG	2.30	0.62
18:T:58:ASN:OD1	18:T:61:LYS:NZ	2.33	0.62
57:o:23:GLN:OE1	57:o:23:GLN:N	2.33	0.62
12:M:144:PHE:O	12:M:147:THR:OG1	2.17	0.62
13:O:34:GLN:OE1	22:D:3:HIS:ND1	2.33	0.62
23:C:13:ARG:NH1	23:C:77:SER:O	2.32	0.62
37:a:1248:U:O2'	37:a:1249:G:O5'	2.17	0.62
57:o:17:LYS:O	57:o:21:ARG:N	2.33	0.62
4:d:58:VAL:HG13	4:d:58:VAL:O	2.00	0.61
9:A:2790:A:N1	19:U:28:SER:OG	2.29	0.61
10:K:20:ASP:O	10:K:22:ALA:N	2.33	0.61
37:a:953:G:HO2'	37:a:1348:G:HO2'	1.48	0.61
3:E:507:G:N2	3:E:567:C:O5'	2.33	0.61
17:S:131:ALA:HA	17:S:141:VAL:HG21	1.82	0.61
37:a:1476:A:OP1	48:n:44:LYS:HD2	1.99	0.61
43:h:50:ALA:O	43:h:54:THR:HG22	2.00	0.61
1:c:51:GLU:O	1:c:51:GLU:HG2	1.99	0.61
5:B:7:G:OP1	22:D:15:ARG:NH2	2.33	0.61
37:a:977:C:H4'	58:9:8:VAL:HG21	1.81	0.61
56:H:35:ILE:HD12	56:H:49:ILE:HA	1.82	0.61
4:d:28:LYS:HZ2	4:d:47:HIS:CE1	2.18	0.61
37:a:637:U:O2	49:p:22:THR:OG1	2.19	0.61
9:A:2188:G:O2'	9:A:2191:C:OP2	2.17	0.61
9:A:3043:G:O2'	9:A:3045:C:OP2	2.18	0.61
37:a:408:G:O2'	40:e:104:ARG:NH2	2.33	0.61
9:A:2537:C:OP1	13:O:75:ARG:NE	2.30	0.61
16:R:41:ARG:NH1	17:S:120:ALA:O	2.33	0.61
39:G:123:LEU:CD1	39:G:129:PHE:HA	2.29	0.61
50:q:39:ARG:NH1	50:q:50:GLN:OE1	2.34	0.61
9:A:2427:G:OP1	10:K:148:ARG:NH1	2.34	0.61
9:A:2538:A:OP1	13:O:95:ARG:NH1	2.33	0.61
9:A:84:U:O2	31:6:45:ARG:NH1	2.33	0.61
10:K:155:LEU:HD13	10:K:177:MET:CE	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:422:A:O2'	12:M:170:ARG:NH2	2.34	0.60
9:A:616:A:OP1	18:T:113:LYS:NZ	2.34	0.60
9:A:2386:U:OP1	9:A:2393:A:O2'	2.12	0.60
3:E:503:C:C4	3:E:572:U:C5	2.88	0.60
9:A:29:C:N4	9:A:535:A:OP2	2.33	0.60
6:j:81:LYS:NZ	37:a:1292:G:OP1	2.26	0.60
9:A:2357:A:C5	9:A:2380:G:N2	2.69	0.60
24:W:50:ARG:O	24:W:54:LYS:NZ	2.32	0.60
37:a:22:C:OP1	41:f:157:ASN:ND2	2.34	0.60
3:E:503:C:H5	3:E:572:U:N3	1.92	0.60
3:E:509:G:O2'	3:E:510:G:N7	2.32	0.60
6:j:96:LEU:O	6:j:110:ARG:NH1	2.35	0.60
9:A:284:G:N2	9:A:302:U:O2	2.33	0.60
37:a:16:U:O2'	37:a:896:A:OP1	2.18	0.60
37:a:426:U:O2'	37:a:427:U:OP1	2.18	0.60
4:d:46:GLY:CA	4:d:61:PHE:CE1	2.82	0.60
9:A:980:C:O2'	9:A:981:U:O5'	2.19	0.60
50:q:44:GLU:OE1	50:q:44:GLU:N	2.34	0.60
9:A:1269:C:O2'	24:W:121:VAL:O	2.15	0.60
43:h:54:THR:HG23	43:h:56:THR:HG22	1.83	0.60
50:q:54:GLU:N	50:q:54:GLU:OE1	2.35	0.60
9:A:2224:C:O2'	9:A:2913:U:OP2	2.20	0.60
39:G:123:LEU:HD11	39:G:129:PHE:CA	2.30	0.60
9:A:1226:U:OP1	16:R:54:ASN:ND2	2.35	0.60
9:A:2091:U:O2'	9:A:2092:U:O4'	2.19	0.60
9:A:2973:A:O2'	14:P:63:ARG:NH1	2.35	0.60
20:V:86:ALA:O	20:V:101:LYS:NZ	2.34	0.60
37:a:1200:A:OP1	58:9:59:ARG:NH1	2.34	0.60
3:E:549:G:O6	3:E:565:U:C2	2.55	0.59
9:A:1640:A:O2'	9:A:1641:U:OP1	2.18	0.59
40:e:145:LEU:O	40:e:154:ARG:NH2	2.35	0.59
4:d:46:GLY:C	4:d:61:PHE:CE1	2.81	0.59
39:G:50:GLY:O	39:G:114:LEU:HD21	2.01	0.59
37:a:501:G:N7	48:n:50:ARG:NH2	2.49	0.59
5:B:99:A:N3	9:A:978:A:O2'	2.36	0.59
37:a:457:A:O2'	37:a:458:A:O4'	2.20	0.59
37:a:1106:U:O4	46:l:9:ARG:NH1	2.35	0.59
11:L:94:GLU:N	11:L:94:GLU:OE1	2.33	0.59
30:4:36:ILE:HD12	30:4:58:THR:HG21	1.84	0.59
1:c:6:ARG:O	1:c:28:ARG:NH2	2.36	0.59
19:U:4:GLN:OE1	19:U:23:ARG:NH2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1229:A:O2'	9:A:1230:G:O4'	2.18	0.59
9:A:191:G:O2'	9:A:792:G:N2	2.35	0.59
9:A:242:G:O2'	9:A:254:G:O6	2.20	0.59
9:A:2173:G:O2'	37:a:1402:G:O2'	2.19	0.59
28:1:45:THR:HG23	28:1:47:VAL:HG12	1.85	0.59
37:a:522:G:OP1	40:e:10:ARG:NH1	2.35	0.59
37:a:1083:C:H5''	53:u:97:LEU:HD22	1.85	0.59
37:a:639:C:OP2	49:p:8:LYS:NZ	2.36	0.58
37:a:1359:U:O4	43:h:10:ARG:NH1	2.36	0.58
37:a:1159:G:N7	45:k:119:LYS:NZ	2.36	0.58
37:a:1199:C:H2'	37:a:1200:A:C8	2.37	0.58
16:R:17:PHE:HD1	16:R:23:THR:HG21	1.69	0.58
56:H:34:THR:HG21	56:H:47:PRO:HG2	1.85	0.58
17:S:34:GLY:O	17:S:66:ARG:NH1	2.36	0.58
37:a:963:U:OP1	58:9:6:LYS:NZ	2.37	0.58
9:A:1598:U:O2'	9:A:1600:G:N7	2.33	0.58
55:I:670:VAL:HG23	55:I:718:PHE:HB2	1.85	0.58
37:a:264:U:O2'	51:r:81:PRO:O	2.18	0.58
29:2:117:ASP:N	29:2:149:GLU:OE1	2.37	0.58
37:a:1329:G:O2'	37:a:1356:G:O6	2.11	0.58
3:E:574:C:N3	9:A:2477:G:N1	2.51	0.58
9:A:1043:G:O2'	32:7:25:THR:O	2.16	0.58
29:2:136:GLU:OE1	29:2:138:LEU:N	2.35	0.58
42:g:4:TYR:CD1	42:g:72:VAL:HG21	2.38	0.58
44:i:12:THR:HG22	44:i:15:ARG:HH12	1.69	0.58
9:A:291:C:O2'	9:A:338:C:OP2	2.12	0.58
9:A:243:U:OP1	35:x:6:THR:OG1	2.13	0.58
9:A:2583:C:O2'	35:x:54:ASP:OD2	2.21	0.58
16:R:21:THR:OG1	16:R:84:GLY:O	2.22	0.58
37:a:666:U:O2'	37:a:667:A:O5'	2.22	0.58
9:A:382:A:OP2	28:1:82:ARG:NH2	2.36	0.57
9:A:1381:G:N7	26:Y:22:THR:OG1	2.28	0.57
12:M:57:GLU:OE2	12:M:94:LYS:NZ	2.35	0.57
37:a:936:G:H21	37:a:1208:A:H62	1.50	0.57
55:I:670:VAL:CG2	55:I:718:PHE:HB2	2.34	0.57
57:o:46:GLU:OE1	57:o:46:GLU:N	2.37	0.57
37:a:324:G:N1	37:a:327:A:OP2	2.36	0.57
37:a:1011:U:O2'	37:a:1012:U:O5'	2.21	0.57
3:E:556:C:O2'	3:E:557:G:O5'	2.23	0.57
4:d:28:LYS:CG	4:d:47:HIS:CE1	2.88	0.57
37:a:148:A:OP2	37:a:166:C:N4	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:u:67:VAL:HG12	53:u:160:ALA:HB3	1.85	0.57
4:d:32:LYS:NZ	4:d:53:ASP:OD1	2.38	0.57
9:A:361:A:N1	9:A:440:U:O2'	2.36	0.57
9:A:2425:U:O2'	9:A:2427:G:OP1	2.21	0.57
37:a:1106:U:OP1	46:l:7:ARG:NH1	2.38	0.57
39:G:86:ILE:CD1	39:G:100:LEU:HD21	2.34	0.57
37:a:20:A:O4'	41:f:47:SER:OG	2.22	0.57
3:E:502:G:N2	9:A:2477:G:H22	2.03	0.57
3:E:503:C:C5	3:E:572:U:O4	2.37	0.57
3:E:504:G:N2	3:E:570:G:H1	2.02	0.57
9:A:2236:G:N7	26:Y:23:LYS:NZ	2.52	0.57
9:A:222:A:O2'	9:A:508:G:N3	2.33	0.57
13:O:113:ILE:HD12	56:H:51:VAL:HG21	1.85	0.57
29:2:8:PRO:HB2	29:2:68:THR:HG23	1.86	0.57
7:N:43:THR:HG22	7:N:94:VAL:HG12	1.87	0.57
10:K:176:ARG:NH2	37:a:692:A:O2'	2.38	0.57
11:L:18:ASP:OD1	11:L:22:LYS:N	2.38	0.57
37:a:761:A:O2'	37:a:1506:U:O2	2.22	0.57
4:d:46:GLY:C	4:d:61:PHE:HE1	2.13	0.56
4:d:55:ARG:CD	37:a:940:A:N7	2.62	0.56
37:a:427:U:O2'	37:a:521:G:OP1	2.23	0.56
52:t:59:ASP:OD1	52:t:76:LYS:NZ	2.38	0.56
56:H:30:THR:O	56:H:34:THR:N	2.38	0.56
7:N:34:ILE:HD12	7:N:104:PHE:HB2	1.87	0.56
37:a:647:G:OP1	37:a:712:C:O2'	2.15	0.56
9:A:114:G:OP2	9:A:116:A:O2'	2.21	0.56
9:A:122:A:N7	34:0:13:ARG:NH1	2.54	0.56
37:a:902:U:O2'	37:a:1061:G:O2'	2.17	0.56
46:l:59:LYS:O	46:l:62:ARG:NE	2.35	0.56
4:d:32:LYS:HB2	55:l:656:ALA:CB	2.35	0.56
9:A:2008:A:N6	9:A:2045:G:O2'	2.35	0.56
9:A:3038:C:OP1	21:J:42:ARG:NH2	2.38	0.56
29:2:109:GLU:OE2	29:2:130:THR:OG1	2.14	0.56
9:A:2388:G:O2'	9:A:2389:U:O4'	2.18	0.56
9:A:2907:C:O2	19:U:76:TYR:OH	2.23	0.56
39:G:94:THR:OG1	39:G:96:LYS:N	2.38	0.56
53:u:111:LEU:HG	53:u:148:LEU:HD23	1.86	0.56
3:E:534:C:O2'	3:E:535:A:OP1	2.10	0.56
12:M:150:GLU:OE1	12:M:150:GLU:N	2.39	0.56
17:S:91:SER:OG	17:S:138:GLY:O	2.23	0.56
39:G:20:SER:OG	39:G:39:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:723:C:O2	9:A:733:U:O2'	2.24	0.56
51:r:67:GLU:N	51:r:67:GLU:OE1	2.39	0.56
4:d:55:ARG:O	4:d:55:ARG:HG3	2.05	0.56
9:A:682:A:OP1	12:M:96:ARG:NH2	2.38	0.56
9:A:1564:A:O2'	9:A:1565:A:O5'	2.24	0.56
13:O:139:LEU:HD13	13:O:144:MET:HE2	1.88	0.56
48:n:98:ILE:O	48:n:101:SER:OG	2.23	0.56
2:y:1:SER:H3	2:y:29:ASP:CB	2.08	0.56
2:y:58:ILE:HG12	2:y:66:VAL:HG11	1.88	0.56
9:A:3052:A:OP1	11:L:60:ARG:NH2	2.39	0.56
37:a:264:U:O2'	51:r:80:ARG:NH1	2.38	0.56
9:A:1542:A:N1	9:A:1543:A:N6	2.54	0.55
9:A:2034:G:OP1	10:K:88:ARG:NH2	2.39	0.55
37:a:1249:G:O2'	37:a:1250:A:O5'	2.23	0.55
9:A:2967:C:OP2	9:A:2979:C:N4	2.39	0.55
37:a:604:U:O2'	50:q:17:GLN:OE1	2.19	0.55
37:a:1298:G:N1	37:a:1301:A:OP2	2.38	0.55
45:k:126:ARG:NH1	45:k:127:ASP:O	2.39	0.55
51:r:92:GLU:N	51:r:92:GLU:OE1	2.39	0.55
53:u:44:GLN:N	53:u:44:GLN:OE1	2.40	0.55
9:A:2070:A:N3	9:A:2457:U:O2'	2.36	0.55
37:a:1044:G:O2'	37:a:1171:G:N2	2.38	0.55
9:A:1578:G:O6	9:A:1593:U:O2	2.23	0.55
40:e:27:GLU:OE1	40:e:27:GLU:N	2.39	0.55
44:i:40:LEU:HD22	44:i:131:VAL:HG21	1.87	0.55
9:A:2329:G:O6	9:A:2407:C:N4	2.40	0.55
9:A:2904:C:O2'	11:L:13:MET:SD	2.65	0.55
20:V:146:GLU:N	20:V:146:GLU:OE1	2.40	0.55
37:a:352:C:O2'	37:a:353:A:O5'	2.25	0.55
21:J:67:MET:HG2	21:J:76:VAL:HG21	1.88	0.55
37:a:983:C:N3	37:a:1019:U:O4	2.39	0.55
4:d:40:ILE:HD11	4:d:71:LEU:HD13	1.88	0.55
9:A:669:G:O2'	9:A:1369:A:OP1	2.24	0.55
17:S:103:THR:O	17:S:107:VAL:HG23	2.07	0.55
3:E:533:U:OP2	45:k:150:ARG:NH1	2.40	0.55
30:4:21:LEU:HD21	30:4:41:ARG:NH1	2.22	0.55
3:E:534:C:HO2'	3:E:535:A:P	2.27	0.54
5:B:67:A:O4'	5:B:106:C:N4	2.40	0.54
9:A:678:A:N1	9:A:924:G:O2'	2.40	0.54
37:a:264:U:O3'	51:r:80:ARG:NH1	2.41	0.54
40:e:159:GLU:OE1	40:e:159:GLU:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:u:61:VAL:HG21	53:u:221:VAL:HG23	1.89	0.54
41:f:204:LEU:O	41:f:208:ALA:HB3	2.07	0.54
51:r:68:ALA:HB2	51:r:93:ILE:HD11	1.88	0.54
56:H:30:THR:CA	56:H:34:THR:HG23	2.38	0.54
3:E:549:G:C6	3:E:565:U:O2	2.59	0.54
17:S:15:ILE:HD11	17:S:58:VAL:HG21	1.88	0.54
9:A:2695:A:OP2	55:I:731:ARG:NH2	2.40	0.54
10:K:262:LYS:N	10:K:265:ASP:OD2	2.39	0.54
9:A:292:G:H22	9:A:343:U:H2'	1.72	0.54
16:R:52:ALA:CB	16:R:79:ILE:HD12	2.38	0.54
29:2:102:ARG:HD3	29:2:138:LEU:HD11	1.89	0.54
37:a:746:A:OP2	37:a:792:G:N2	2.41	0.54
55:I:719:LEU:HD22	55:I:767:GLU:HA	1.89	0.54
9:A:290:C:O2	9:A:300:G:O2'	2.26	0.54
9:A:1675:U:C4	21:J:67:MET:HE1	2.42	0.54
9:A:2091:U:O2'	9:A:2092:U:O5'	2.24	0.54
37:a:544:C:C4	51:r:48:LEU:HD11	2.43	0.54
4:d:44:PHE:CD2	4:d:49:PHE:HE2	2.26	0.54
9:A:1518:A:HO2'	9:A:1692:G:HO2'	1.54	0.54
9:A:2743:U:O4'	9:A:2766:A:N6	2.41	0.54
9:A:2796:A:OP2	11:L:156:THR:N	2.39	0.54
14:P:11:VAL:HG13	14:P:15:VAL:HG11	1.89	0.54
9:A:191:G:O6	9:A:202:C:O2'	2.17	0.54
9:A:569:G:OP2	28:1:44:HIS:ND1	2.41	0.54
9:A:1624:U:O2'	9:A:1625:G:O5'	2.14	0.54
9:A:2367:G:O2'	9:A:2369:C:OP2	2.15	0.54
9:A:2879:G:O2'	9:A:2888:G:O6	2.22	0.54
22:D:9:ASN:OD1	22:D:10:ILE:N	2.41	0.54
39:G:69:THR:HG21	39:G:75:VAL:CG2	2.37	0.54
45:k:46:GLY:N	45:k:79:ASP:OD1	2.41	0.54
9:A:1363:G:OP1	24:W:2:ALA:N	2.41	0.54
9:A:1911:U:O2'	10:K:14:ARG:NH1	2.41	0.54
9:A:2754:G:O2'	9:A:2756:G:OP2	2.11	0.54
39:G:99:GLN:NE2	39:G:101:ASN:OD1	2.41	0.54
46:l:32:THR:HG23	46:l:83:THR:HG22	1.88	0.54
16:R:100:ASN:OD1	16:R:101:LYS:N	2.41	0.53
29:2:165:PRO:HD2	29:2:168:VAL:HG21	1.90	0.53
37:a:1237:C:OP2	37:a:1260:A:N6	2.41	0.53
40:e:188:VAL:HG22	40:e:189:PRO:HD2	1.89	0.53
2:y:34:ASN:ND2	9:A:2424:C:OP1	2.41	0.53
9:A:670:A:OP1	9:A:1370:U:O2'	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:6:ILE:HD13	25:X:41:LEU:HB3	1.91	0.53
40:e:183:ARG:NH1	40:e:183:ARG:O	2.41	0.53
46:l:50:CYS:SG	46:l:62:ARG:NH1	2.81	0.53
40:e:143:LYS:O	40:e:147:THR:HG23	2.09	0.53
48:n:74:LEU:HD21	48:n:104:THR:CG2	2.39	0.53
57:o:24:LEU:HD13	57:o:32:ILE:CD1	2.39	0.53
55:I:668:THR:CB	55:I:718:PHE:CD1	2.91	0.53
9:A:2367:G:N2	9:A:2369:C:O2	2.42	0.53
9:A:2971:G:OP1	14:P:75:ASN:ND2	2.41	0.53
39:G:123:LEU:HD21	39:G:129:PHE:N	2.23	0.53
4:d:44:PHE:CE2	4:d:49:PHE:HZ	2.15	0.53
9:A:473:C:O2'	9:A:476:G:N2	2.42	0.53
9:A:2344:G:O3'	9:A:2392:A:O2'	2.26	0.53
10:K:41:GLY:O	10:K:43:ARG:NH1	2.41	0.53
1:c:14:THR:N	1:c:50:ARG:O	2.42	0.53
9:A:381:A:OP2	28:l:82:ARG:NH1	2.40	0.53
25:X:30:GLU:OE1	25:X:30:GLU:N	2.42	0.53
2:y:58:ILE:HD11	2:y:66:VAL:HG21	1.91	0.53
9:A:886:G:HO2'	9:A:1470:G:HO2'	1.57	0.53
9:A:1493:A:O2'	9:A:1495:G:N7	2.38	0.53
17:S:93:GLU:HG3	55:I:778:LEU:HD23	1.90	0.53
3:E:503:C:C5	3:E:572:U:C6	2.90	0.53
4:d:15:LEU:HD23	4:d:15:LEU:O	2.08	0.53
4:d:57:HIS:CD2	4:d:59:PRO:HG3	2.44	0.53
9:A:667:A:OP2	9:A:2723:C:O2'	2.19	0.53
9:A:1003:A:O2'	9:A:1004:C:O5'	2.13	0.53
9:A:1441:C:HO2'	9:A:2234:G:HO2'	1.53	0.53
28:l:88:ASP:O	28:l:92:GLY:N	2.42	0.53
41:f:63:ILE:HG21	41:f:139:VAL:HA	1.91	0.53
9:A:17:C:OP1	24:W:22:LYS:NZ	2.42	0.52
11:L:88:ASP:OD1	11:L:88:ASP:N	2.40	0.52
2:y:13:PHE:CE2	2:y:27:ARG:HD2	2.43	0.52
4:d:55:ARG:HD2	37:a:940:A:C8	2.43	0.52
37:a:1331:A:OP2	45:k:140:LYS:NZ	2.41	0.52
40:e:185:GLN:N	40:e:185:GLN:OE1	2.42	0.52
43:h:64:ARG:NE	43:h:128:SER:OG	2.43	0.52
45:k:87:LEU:HD12	45:k:95:GLN:HB3	1.91	0.52
6:j:84:ILE:HG21	55:I:681:ARG:HD2	1.90	0.52
37:a:497:G:O2'	37:a:511:U:O5'	2.16	0.52
41:f:104:SER:OG	41:f:146:HIS:ND1	2.40	0.52
44:i:40:LEU:CD2	44:i:131:VAL:HG21	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:44:C:O2	13:O:99:ARG:NE	2.32	0.52
9:A:2515:U:O2'	9:A:2598:C:O2	2.26	0.52
21:J:5:THR:OG1	21:J:17:GLN:NE2	2.40	0.52
37:a:599:U:N3	40:e:126:ASP:OD1	2.43	0.52
44:i:18:ASN:O	44:i:72:ARG:NH1	2.41	0.52
26:Y:65:ALA:HB1	26:Y:71:LEU:HD12	1.91	0.52
37:a:99:U:OP2	52:t:9:LYS:NZ	2.26	0.52
58:9:2:ALA:N	58:9:67:ASP:O	2.43	0.52
9:A:249:C:O2	35:x:12:LYS:NZ	2.36	0.52
9:A:2796:A:P	11:L:156:THR:HB	2.50	0.52
9:A:2842:G:H21	11:L:160:VAL:HG21	1.74	0.52
37:a:823:U:O4	37:a:826:U:N3	2.42	0.52
3:E:556:C:O2'	3:E:557:G:O4'	2.27	0.52
4:d:33:THR:HG23	4:d:51:VAL:HG12	1.91	0.52
9:A:1003:A:HO2'	9:A:1004:C:P	2.30	0.52
9:A:296:A:N1	9:A:340:A:N6	2.58	0.52
9:A:2216:G:N2	9:A:2220:C:O2'	2.43	0.52
37:a:439:U:O2'	40:e:114:SER:O	2.17	0.52
9:A:1000:C:OP1	9:A:1002:C:N4	2.43	0.52
37:a:1047:A:N1	37:a:1088:G:O2'	2.36	0.52
41:f:64:VAL:HG12	41:f:92:ALA:HB1	1.91	0.52
9:A:1401:A:O2'	9:A:1403:C:OP2	2.26	0.51
4:d:45:ILE:O	4:d:62:VAL:C	2.49	0.51
9:A:2371:G:O2'	9:A:2372:U:O5'	2.28	0.51
19:U:104:ARG:NH2	19:U:121:VAL:O	2.43	0.51
20:V:64:LEU:HD23	35:x:25:GLN:HG3	1.91	0.51
21:J:33:ARG:NH2	21:J:114:GLU:OE1	2.43	0.51
44:i:63:GLN:N	44:i:63:GLN:OE1	2.42	0.51
4:d:36:ARG:HH11	4:d:36:ARG:HG2	1.75	0.51
9:A:619:C:O2	24:W:28:ARG:NH2	2.43	0.51
37:a:91:U:HO2'	37:a:92:A:P	2.31	0.51
53:u:200:ILE:HG21	53:u:213:LEU:HD12	1.92	0.51
37:a:1303:U:OP2	37:a:1304:C:O2'	2.24	0.51
9:A:1947:U:O2'	9:A:1948:A:O4'	2.28	0.51
1:c:11:LEU:HD12	1:c:25:LYS:CA	2.41	0.51
1:c:14:THR:O	1:c:50:ARG:N	2.43	0.51
3:E:503:C:C4	3:E:572:U:C6	2.99	0.51
32:7:38:GLU:O	32:7:43:THR:HG21	2.11	0.51
37:a:11:G:H22	41:f:122:ARG:CZ	2.24	0.51
40:e:98:TYR:O	40:e:160:ARG:NH2	2.42	0.51
53:u:167:ASN:ND2	53:u:190:ASN:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:y:44:ARG:NH2	9:A:2441:G:O2'	2.42	0.51
37:a:672:U:O2'	37:a:674:G:N7	2.27	0.51
1:c:7:PRO:O	1:c:28:ARG:N	2.40	0.51
3:E:503:C:H2'	3:E:503:C:O2	2.10	0.51
9:A:249:C:OP2	9:A:2618:C:O2'	2.23	0.51
9:A:908:A:OP2	9:A:2294:A:O2'	2.17	0.51
9:A:2474:G:N2	9:A:2500:G:OP1	2.43	0.51
37:a:461:G:O2'	37:a:463:C:N4	2.40	0.51
47:m:64:SER:O	47:m:67:SER:OG	2.29	0.51
21:J:26:THR:HG23	21:J:75:VAL:HG21	1.92	0.51
37:a:145:G:O2'	37:a:1429:A:N3	2.40	0.51
53:u:184:ILE:HG22	53:u:198:TYR:HB2	1.91	0.51
56:H:30:THR:HG23	56:H:32:THR:H	1.75	0.51
9:A:1182:C:N4	9:A:1187:A:O2'	2.44	0.50
9:A:1675:U:N3	21:J:67:MET:HE1	2.25	0.50
9:A:2537:C:O4'	13:O:44:ASN:ND2	2.44	0.50
58:9:64:ASP:OD1	58:9:65:VAL:N	2.44	0.50
5:B:7:G:O3'	22:D:41:ASN:ND2	2.43	0.50
37:a:1132:U:H5''	46:l:44:THR:HG23	1.92	0.50
40:e:71:TYR:HE1	40:e:196:VAL:HG23	1.77	0.50
1:c:11:LEU:CD2	1:c:26:ASN:HB3	2.41	0.50
4:d:56:LYS:HD3	55:I:660:LEU:HD11	1.91	0.50
37:a:1199:C:O2'	37:a:1200:A:H5'	2.12	0.50
9:A:389:G:N1	9:A:392:A:OP2	2.39	0.50
42:g:96:HIS:O	42:g:96:HIS:ND1	2.44	0.50
44:i:80:VAL:HG12	44:i:87:VAL:HG21	1.92	0.50
2:y:37:TYR:CD2	2:y:48:LEU:HD12	2.46	0.50
53:u:161:VAL:HB	53:u:183:VAL:HG12	1.93	0.50
9:A:2473:U:N3	9:A:2477:G:OP2	2.42	0.50
20:V:51:GLU:OE2	35:x:57:ARG:NH1	2.42	0.50
6:j:49:THR:N	6:j:52:GLN:OE1	2.43	0.50
28:1:86:ARG:NH2	28:1:104:ASP:OD2	2.45	0.50
9:A:2469:U:O2'	9:A:2660:G:OP2	2.25	0.50
29:2:72:GLU:N	29:2:72:GLU:OE1	2.44	0.50
37:a:1232:A:N3	37:a:1352:C:O2'	2.35	0.50
43:h:20:SER:HB3	43:h:23:VAL:HG12	1.93	0.50
55:I:696:GLU:OE1	55:I:696:GLU:N	2.42	0.50
9:A:860:G:HO2'	9:A:863:G:HO2'	1.58	0.50
9:A:1206:A:N7	17:S:136:SER:OG	2.33	0.50
9:A:1542:A:N6	9:A:1628:A:O3'	2.45	0.50
9:A:1001:C:O2'	55:I:701:GLN:NE2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:a:821:C:N4	37:a:823:U:O4	2.41	0.49
40:e:9:THR:O	40:e:12:SER:OG	2.23	0.49
46:l:5:LYS:HB3	46:l:77:LEU:HD13	1.94	0.49
46:l:80:THR:O	46:l:83:THR:OG1	2.22	0.49
4:d:45:ILE:CA	4:d:62:VAL:HG13	2.42	0.49
9:A:79:G:N1	9:A:100:A:OP2	2.44	0.49
9:A:403:U:O2'	9:A:422:A:N3	2.46	0.49
9:A:1456:G:OP1	9:A:1512:U:N3	2.41	0.49
9:A:2044:U:O2'	9:A:2194:A:N3	2.40	0.49
17:S:77:ALA:HB1	17:S:130:ILE:HG23	1.94	0.49
50:q:21:ILE:HG22	50:q:36:VAL:HG22	1.93	0.49
53:u:81:ALA:O	53:u:85:THR:HG23	2.12	0.49
55:l:733:LEU:O	55:l:736:VAL:HG12	2.12	0.49
5:B:81:U:O2'	9:A:1033:A:N3	2.44	0.49
5:B:106:C:O2'	5:B:107:A:OP2	2.25	0.49
39:G:34:GLU:OE2	39:G:58:ARG:NH1	2.46	0.49
4:d:33:THR:HG23	4:d:33:THR:O	2.12	0.49
12:M:178:ILE:HD11	12:M:182:GLN:O	2.12	0.49
37:a:996:G:O6	58:9:50:ARG:NH1	2.45	0.49
37:a:1420:C:OP1	52:t:29:ARG:NH2	2.46	0.49
2:y:38:TYR:O	2:y:63:ILE:HG21	2.12	0.49
4:d:44:PHE:HE2	4:d:49:PHE:CE2	2.24	0.49
9:A:284:G:O2'	9:A:286:G:O4'	2.31	0.49
15:Q:85:ALA:HB2	15:Q:92:PHE:HE1	1.77	0.49
2:y:1:SER:N	2:y:29:ASP:CB	2.71	0.49
11:L:37:THR:HG21	11:L:70:PHE:CE1	2.48	0.49
32:7:2:ALA:O	32:7:39:ASP:N	2.46	0.49
37:a:737:U:O2'	37:a:861:C:O2	2.29	0.49
9:A:1479:G:N2	9:A:1482:A:OP2	2.39	0.49
19:U:24:VAL:HG13	19:U:33:ALA:HB2	1.94	0.49
37:a:1199:C:C2	37:a:1200:A:C8	3.01	0.49
37:a:1200:A:H2'	37:a:1201:G:C8	2.47	0.49
9:A:3020:U:O2'	9:A:3021:A:O5'	2.29	0.49
11:L:89:GLU:HA	11:L:92:VAL:HG12	1.94	0.49
37:a:10:G:HO2'	37:a:11:G:P	2.36	0.49
9:A:2528:G:N2	13:O:160:ASP:OD2	2.46	0.49
39:G:50:GLY:C	39:G:114:LEU:HD21	2.38	0.49
3:E:541:C:O2	3:E:542:A:N6	2.42	0.48
9:A:921:C:O2	9:A:2668:G:O2'	2.31	0.48
9:A:1200:U:O2'	16:R:40:ARG:NE	2.46	0.48
9:A:2764:C:O2'	9:A:2964:A:N3	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:65:ALA:O	56:H:28:THR:HG21	2.13	0.48
17:S:10:LEU:HD22	17:S:61:THR:HG22	1.94	0.48
37:a:37:A:N3	48:n:29:GLN:NE2	2.56	0.48
40:e:144:SER:O	40:e:147:THR:OG1	2.29	0.48
55:I:667:CYS:O	55:I:668:THR:OG1	2.30	0.48
9:A:2385:G:OP2	9:A:2387:U:N3	2.43	0.48
53:u:117:LEU:HD13	53:u:141:LYS:HG3	1.95	0.48
55:I:727:LEU:HD22	55:I:732:LEU:HD12	1.94	0.48
3:E:518(B):G:O6	13:O:86:LEU:N	2.46	0.48
5:B:2:U:O2'	5:B:3:U:OP1	2.25	0.48
9:A:860:G:O2'	9:A:863:G:O2'	2.29	0.48
9:A:1180:G:N2	17:S:136:SER:O	2.47	0.48
37:a:749:G:OP2	37:a:783:G:O2'	2.27	0.48
41:f:130:VAL:N	41:f:146:HIS:O	2.47	0.48
55:I:756:ASN:ND2	55:I:759:VAL:O	2.44	0.48
55:I:757:ASP:OD1	55:I:761:ILE:HD11	2.13	0.48
13:O:141:GLU:OE1	13:O:143:SER:OG	2.29	0.48
22:D:9:ASN:OD1	22:D:10:ILE:HG22	2.12	0.48
37:a:544:C:C5	51:r:48:LEU:HD11	2.49	0.48
37:a:791:C:O2'	37:a:883:A:N1	2.44	0.48
55:I:778:LEU:HD21	55:I:790:VAL:HB	1.95	0.48
4:d:46:GLY:CA	4:d:61:PHE:HE1	2.26	0.48
9:A:2973:A:O3'	14:P:63:ARG:NH1	2.47	0.48
17:S:77:ALA:CB	17:S:130:ILE:HD12	2.43	0.48
32:7:43:THR:HA	32:7:46:LEU:HD12	1.96	0.48
53:u:18:HIS:NE2	53:u:188:ASP:OD2	2.46	0.48
9:A:218:A:N3	9:A:234:U:O2'	2.41	0.48
37:a:1220:A:H62	37:a:1281:A:N6	2.12	0.48
55:I:784:VAL:HG13	55:I:786:GLY:H	1.79	0.48
7:N:128:LYS:NZ	9:A:1147:A:OP1	2.39	0.48
9:A:589:A:O2'	9:A:592:A:OP1	2.16	0.48
36:F:16:VAL:HG22	36:F:25:VAL:HG22	1.95	0.48
37:a:13:G:OP2	41:f:151:LYS:NZ	2.45	0.48
51:r:42:ASP:OD1	51:r:42:ASP:N	2.45	0.48
3:E:501:C:O2	3:E:501:C:O2'	2.26	0.48
5:B:7:G:OP1	5:B:29:C:O2'	2.31	0.48
9:A:571:A:O2'	28:1:45:THR:O	2.24	0.48
37:a:10:G:O2'	37:a:11:G:O5'	2.24	0.48
3:E:518(B):G:N1	13:O:82:ALA:O	2.45	0.48
4:d:32:LYS:NZ	4:d:53:ASP:CG	2.71	0.48
9:A:1330:C:OP1	24:W:15:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2031:G:OP2	9:A:2032:A:O2'	2.20	0.48
2:y:2:ALA:HB3	2:y:32:ILE:HG21	1.96	0.48
10:K:2:GLY:N	10:K:20:ASP:OD1	2.47	0.48
32:7:46:LEU:O	32:7:50:VAL:HG22	2.14	0.48
37:a:821:C:N4	37:a:822:U:O2	2.47	0.48
37:a:969:G:N1	37:a:1200:A:C6	2.82	0.48
53:u:107:VAL:HG13	53:u:148:LEU:HD21	1.95	0.48
58:9:53:ARG:O	58:9:56:SER:OG	2.32	0.48
3:E:504:G:N3	3:E:570:G:O6	2.47	0.47
9:A:1002:C:OP2	55:I:681:ARG:N	2.47	0.47
14:P:114:VAL:HG11	14:P:152:LEU:HD22	1.96	0.47
37:a:64:A:OP1	37:a:107:G:N2	2.46	0.47
58:9:36:SER:O	58:9:36:SER:OG	2.30	0.47
9:A:1552:A:N6	9:A:1616:A:OP2	2.47	0.47
26:Y:37:GLU:OE1	26:Y:37:GLU:N	2.44	0.47
37:a:519:A:OP2	48:n:112:GLN:NE2	2.47	0.47
4:d:50:ALA:CB	4:d:57:HIS:CE1	2.97	0.47
5:B:83:C:OP1	32:7:16:ARG:NH1	2.45	0.47
9:A:2074:G:O2'	9:A:2109:A:N6	2.45	0.47
16:R:52:ALA:HB2	16:R:79:ILE:HD12	1.95	0.47
22:D:80:HIS:O	22:D:84:VAL:HG23	2.14	0.47
37:a:1248:U:O2'	37:a:1249:G:O4'	2.32	0.47
39:G:65:VAL:O	39:G:67:ILE:HG23	2.15	0.47
3:E:565:U:O2'	3:E:566:C:OP1	2.32	0.47
16:R:52:ALA:HB3	16:R:77:THR:CG2	2.43	0.47
34:0:34:VAL:HG13	34:0:45:LEU:HD13	1.96	0.47
37:a:413:G:H22	37:a:429:U:P	2.37	0.47
46:l:28:THR:OG1	46:l:31:ARG:NH2	2.47	0.47
4:d:18:LYS:HD3	4:d:31:ILE:HG23	1.97	0.47
10:K:26:ARG:NH2	10:K:83:GLU:OE2	2.47	0.47
20:V:105:ARG:O	20:V:108:SER:OG	2.32	0.47
53:u:97:LEU:H	53:u:100:MET:HE3	1.78	0.47
9:A:1175:A:O2'	16:R:34:ALA:HB2	2.15	0.47
9:A:2340:A:N7	9:A:2394:A:N6	2.56	0.47
29:2:143:GLN:O	29:2:144:LEU:HD22	2.15	0.47
50:q:77:THR:OG1	50:q:79:ASP:OD2	2.27	0.47
55:I:745:VAL:HG11	55:I:765:THR:HG23	1.96	0.47
2:y:58:ILE:CD1	2:y:66:VAL:HG21	2.45	0.47
9:A:15:C:O2'	9:A:646:U:OP1	2.30	0.47
9:A:273:A:H62	9:A:313:G:N2	2.13	0.47
9:A:2016:G:O2'	10:K:181:GLU:OE2	2.16	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2795:C:O2'	11:L:156:THR:CG2	2.63	0.47
16:R:43:LEU:HD22	16:R:92:ALA:HB1	1.97	0.47
29:2:132:GLU:HB2	29:2:171:ILE:HD11	1.96	0.47
49:p:66:LEU:O	49:p:70:VAL:HG23	2.15	0.47
53:u:1:MET:SD	53:u:1:MET:N	2.82	0.47
9:A:2334:U:N3	9:A:2368:C:O2'	2.46	0.47
9:A:2663:A:O2'	9:A:2824:A:OP1	2.23	0.47
37:a:20:A:C4'	41:f:47:SER:HG	2.28	0.47
37:a:761:A:OP1	47:m:134:LYS:NZ	2.46	0.47
37:a:1220:A:H62	37:a:1281:A:H61	1.63	0.47
44:i:5:ASP:OD2	44:i:5:ASP:N	2.48	0.47
44:i:39:ILE:HG21	44:i:105:ILE:HD12	1.95	0.47
9:A:240:G:O2'	9:A:257:A:N6	2.43	0.47
3:E:528:U:H3	3:E:541:C:H42	1.64	0.47
9:A:49:A:OP2	9:A:116:A:N6	2.48	0.47
29:2:4:THR:O	29:2:139:SER:OG	2.19	0.47
37:a:66:U:O2'	37:a:379:C:O2	2.32	0.47
37:a:1053:U:O2	53:u:103:ASN:ND2	2.48	0.47
9:A:2581:G:O2'	9:A:2583:C:OP2	2.17	0.46
39:G:86:ILE:HD12	39:G:100:LEU:HD21	1.96	0.46
55:I:675:ILE:HD11	55:I:710:TRP:HB2	1.97	0.46
2:y:13:PHE:CE2	2:y:27:ARG:CG	2.98	0.46
4:d:37:ARG:O	4:d:37:ARG:HG2	2.14	0.46
5:B:82:A:H2	5:B:94:G:H22	1.63	0.46
12:M:50:HIS:NE2	12:M:98:TYR:OH	2.38	0.46
39:G:69:THR:HG22	39:G:71:ARG:H	1.80	0.46
48:n:74:LEU:HD21	48:n:104:THR:HG22	1.98	0.46
13:O:112:SER:O	13:O:113:ILE:HD13	2.14	0.46
2:y:62:GLY:O	2:y:66:VAL:HG12	2.16	0.46
6:j:3:ARG:C	6:j:4:LEU:HD12	2.40	0.46
14:P:149:ILE:HG22	14:P:163:VAL:HG11	1.97	0.46
29:2:54:PHE:CE2	29:2:58:LEU:HD11	2.51	0.46
37:a:100:G:OP1	52:t:16:ARG:NH1	2.48	0.46
9:A:779:U:O2'	9:A:1058:A:OP2	2.30	0.46
9:A:813:C:O2'	9:A:849:A:N6	2.49	0.46
9:A:828:G:OP2	49:p:88:ARG:NH2	2.48	0.46
9:A:1086:C:OP2	32:7:16:ARG:NE	2.48	0.46
21:J:70:ILE:HG22	21:J:72:ASP:H	1.80	0.46
37:a:874:A:HO2'	37:a:1398:G:HO2'	1.63	0.46
9:A:587:G:N1	9:A:590:A:OP2	2.45	0.46
9:A:2178:G:O2'	9:A:2180:U:O4	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:32:LYS:CB	55:I:656:ALA:CB	2.94	0.46
5:B:71:C:H42	5:B:105:A:H61	1.63	0.46
6:j:87:TYR:OH	6:j:91:ARG:NH2	2.49	0.46
9:A:2796:A:OP2	11:L:156:THR:CB	2.62	0.46
47:m:44:THR:HG22	47:m:50:VAL:HG22	1.98	0.46
4:d:10:PHE:O	4:d:39:THR:HG22	2.16	0.46
9:A:159:A:N3	9:A:2431:C:O2'	2.41	0.46
37:a:1080:C:OP2	53:u:95:ARG:NH1	2.46	0.46
6:j:15:MET:HG3	6:j:34:LEU:HD21	1.98	0.46
9:A:1107:G:OP2	32:7:11:SER:OG	2.25	0.46
9:A:2882:C:P	14:P:161:LYS:HZ1	2.38	0.46
37:a:362:G:N1	37:a:365:U:OP2	2.43	0.46
53:u:41:ILE:HG21	53:u:201:PRO:O	2.15	0.46
6:j:28:THR:HG21	37:a:1310:C:H5''	1.98	0.46
9:A:731:A:OP1	20:V:132:SER:OG	2.28	0.46
9:A:1201:G:N2	9:A:1204:A:OP2	2.49	0.46
9:A:2189:C:OP1	9:A:2190:A:O2'	2.31	0.46
9:A:2788:A:OP1	9:A:2872:G:O2'	2.34	0.46
26:Y:72:ASP:OD1	26:Y:74:SER:OG	2.33	0.46
9:A:273:A:H62	9:A:313:G:H21	1.64	0.45
10:K:83:GLU:OE1	10:K:104:TYR:OH	2.19	0.45
11:L:5:GLY:HA3	11:L:84:LEU:HD21	1.97	0.45
37:a:296:U:O2'	37:a:536:C:O2	2.31	0.45
9:A:1174:G:H2'	9:A:1220:C:H41	1.81	0.45
9:A:2909:G:OP1	23:C:48:ARG:NH1	2.45	0.45
9:A:3118:U:O2	18:T:134:ALA:HB1	2.16	0.45
13:O:47:VAL:HG23	13:O:47:VAL:O	2.17	0.45
29:2:17:THR:OG1	29:2:18:ARG:N	2.49	0.45
37:a:1297:U:O2'	37:a:1342:A:N3	2.31	0.45
42:g:76:ASP:OD1	42:g:88:THR:HG21	2.16	0.45
9:A:933:G:N1	9:A:1303:U:OP2	2.46	0.45
9:A:2864:G:OP1	18:T:87:ARG:NH2	2.45	0.45
18:T:30:SER:O	18:T:34:THR:OG1	2.30	0.45
31:6:22:LEU:HD11	31:6:54:ILE:HG23	1.98	0.45
37:a:1168:G:H21	58:9:100:SER:HB3	1.81	0.45
40:e:23:ASP:N	40:e:23:ASP:OD1	2.48	0.45
53:u:199:PRO:C	53:u:200:ILE:HD12	2.42	0.45
3:E:504:G:H2'	3:E:570:G:O6	2.16	0.45
13:O:83:GLN:OE1	13:O:83:GLN:N	2.45	0.45
18:T:45:THR:HG22	18:T:47:ASN:OD1	2.17	0.45
32:7:40:ASN:OD1	32:7:43:THR:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:a:420:U:O2'	37:a:423:G:O6	2.27	0.45
37:a:1177:A:O2'	37:a:1178:A:OP1	2.22	0.45
48:n:114:ARG:HB3	48:n:119:ALA:HB3	1.98	0.45
10:K:136:ILE:O	10:K:168:LYS:NZ	2.49	0.45
13:O:29:TYR:CD2	13:O:35:ILE:HD13	2.52	0.45
16:R:52:ALA:HB3	16:R:77:THR:HG22	1.98	0.45
37:a:75:A:H61	37:a:95:C:H1'	1.82	0.45
37:a:407:A:OP1	40:e:107:ARG:NH1	2.50	0.45
40:e:41:ILE:HG22	40:e:43:GLU:H	1.82	0.45
44:i:3:MET:HE1	44:i:9:ASP:HB2	1.99	0.45
9:A:357:U:O4	9:A:364:A:N6	2.50	0.45
12:M:2:THR:OG1	12:M:19:GLU:OE2	2.25	0.45
14:P:102:GLN:OE1	14:P:102:GLN:N	2.45	0.45
3:E:576:A:OP1	9:A:2663:A:N6	2.50	0.45
6:j:14:ARG:NH2	6:j:16:GLU:OE2	2.50	0.45
9:A:164:A:N7	15:Q:121:LYS:NZ	2.65	0.45
9:A:324:C:N4	9:A:451:U:O4	2.50	0.45
9:A:639:C:O2'	9:A:640:G:OP2	2.26	0.45
9:A:1550:G:N2	9:A:1620:U:O2	2.49	0.45
9:A:2772:G:O2'	19:U:4:GLN:OE1	2.29	0.45
9:A:2925:C:H3'	9:A:2926:A:H5''	1.99	0.45
17:S:78:ALA:HB1	17:S:137:MET:CE	2.47	0.45
37:a:969:G:C6	37:a:1200:A:N6	2.85	0.45
39:G:110:SER:OG	39:G:204:LYS:NZ	2.34	0.45
3:E:505:G:N2	3:E:506:G:N7	2.61	0.45
4:d:9:PRO:HB3	4:d:39:THR:HG21	1.99	0.45
4:d:56:LYS:HD3	55:I:660:LEU:CD1	2.46	0.45
4:d:58:VAL:HG21	4:d:75:ALA:HA	1.99	0.45
7:N:27:VAL:HG22	7:N:105:GLU:OE2	2.17	0.45
9:A:1000:C:O2	55:I:694:ASN:ND2	2.50	0.45
14:P:99:LEU:HD12	14:P:103:ASN:O	2.17	0.45
40:e:182:GLU:O	40:e:185:GLN:N	2.50	0.45
41:f:182:ARG:NE	44:i:43:GLU:O	2.47	0.45
9:A:1182:C:O2'	55:I:780:VAL:HG23	2.17	0.45
14:P:35:LEU:HD13	14:P:73:ILE:HD13	1.98	0.45
23:C:81:ASP:OD2	23:C:82:HIS:ND1	2.48	0.45
40:e:54:GLN:OE1	40:e:57:ARG:NH1	2.49	0.45
55:I:735:ASP:O	55:I:739:VAL:HG22	2.17	0.45
58:9:67:ASP:OD1	58:9:67:ASP:N	2.46	0.45
6:j:27:ARG:O	6:j:31:ASN:ND2	2.49	0.45
11:L:115:THR:HG21	11:L:174:ARG:CZ	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:86:LEU:HD12	13:O:90:MET:SD	2.57	0.45
18:T:13:ARG:NH2	18:T:49:ASP:O	2.50	0.45
24:W:89:GLU:O	25:X:13:GLN:NE2	2.45	0.45
30:4:36:ILE:HD12	30:4:58:THR:CG2	2.47	0.45
9:A:663:A:O2'	9:A:665:G:O5'	2.35	0.44
27:Z:4:ILE:CG1	31:6:22:LEU:HD23	2.47	0.44
39:G:150:ARG:NH1	39:G:152:GLN:OE1	2.46	0.44
44:i:131:VAL:HG22	44:i:131:VAL:O	2.16	0.44
2:y:38:TYR:C	2:y:39:LEU:HD12	2.43	0.44
9:A:947:U:OP2	9:A:1061:G:N1	2.42	0.44
9:A:1073:G:O6	9:A:1075:U:O2'	2.35	0.44
19:U:80:ASP:OD2	23:C:61:ARG:NH2	2.47	0.44
31:6:28:GLU:OE2	31:6:46:ARG:NH2	2.50	0.44
37:a:101:G:OP1	52:t:17:ARG:NH2	2.50	0.44
53:u:113:ARG:NH2	53:u:117:LEU:HD21	2.32	0.44
9:A:1162:G:H5''	16:R:1:MET:HE1	2.00	0.44
9:A:891:G:N2	9:A:2465:A:OP1	2.47	0.44
9:A:944:A:N7	9:A:2471:A:O2'	2.50	0.44
32:7:21:GLU:OE1	32:7:24:ARG:NH2	2.47	0.44
36:F:8:LYS:O	36:F:34:GLN:NE2	2.50	0.44
39:G:37:ALA:HB3	39:G:93:LEU:HD21	1.99	0.44
4:d:44:PHE:O	4:d:44:PHE:CD2	2.70	0.44
7:N:50:ALA:HB1	7:N:121:ALA:HB1	2.00	0.44
9:A:1391:G:OP2	9:A:1863:G:O2'	2.32	0.44
9:A:2693:A:N6	9:A:2705:G:O2'	2.50	0.44
13:O:67:ILE:O	13:O:109:ARG:NH1	2.45	0.44
28:1:7:ASP:OD2	28:1:96:ARG:NH1	2.46	0.44
9:A:659:U:OP2	20:V:31:LYS:NZ	2.42	0.44
9:A:1974:A:O2'	9:A:1975:A:OP1	2.29	0.44
14:P:99:LEU:HD11	14:P:101:GLY:O	2.18	0.44
15:Q:26:GLY:O	15:Q:31:LEU:HD13	2.17	0.44
22:D:46:HIS:O	22:D:112:ARG:NH2	2.50	0.44
37:a:1040:U:OP1	58:9:85:ARG:NH2	2.50	0.44
37:a:1203:G:OP2	37:a:1304:C:N4	2.49	0.44
55:I:668:THR:CB	55:I:718:PHE:HD1	2.30	0.44
56:H:27:SER:OG	56:H:29:ALA:O	2.35	0.44
57:o:22:ASN:ND2	57:o:25:GLU:OE1	2.51	0.44
6:j:5:VAL:HG13	6:j:6:GLY:H	1.83	0.44
6:j:50:ASP:O	6:j:54:THR:HG23	2.17	0.44
7:N:56:ARG:HE	55:I:729:ARG:CB	2.30	0.44
9:A:789:G:H2'	9:A:919:A:H61	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:928:U:O2'	9:A:1339:G:O2'	2.18	0.44
9:A:1110:C:OP1	24:W:47:TYR:OH	2.23	0.44
9:A:2800:G:O2'	9:A:2803:C:OP2	2.28	0.44
26:Y:14:ALA:HB2	26:Y:57:VAL:HG22	2.00	0.44
9:A:136:U:N3	9:A:139:U:OP2	2.44	0.44
9:A:1177:G:O2'	17:S:118:LEU:HD11	2.18	0.44
26:Y:44:ARG:NH2	33:8:53:ASP:O	2.43	0.44
27:Z:4:ILE:HG13	31:6:22:LEU:HD23	2.00	0.44
37:a:139:C:O2'	37:a:210:A:N1	2.46	0.44
37:a:560:C:H2'	37:a:561:G:O4'	2.17	0.44
39:G:123:LEU:CD2	39:G:129:PHE:HB3	2.40	0.44
48:n:87:VAL:HG11	48:n:90:LEU:HD12	1.99	0.44
49:p:32:LEU:HD22	49:p:59:LEU:HD22	1.99	0.44
37:a:401:C:O2'	37:a:601:A:N3	2.38	0.44
39:G:123:LEU:HD11	39:G:129:PHE:CB	2.48	0.44
9:A:392:A:O2'	9:A:393:U:OP2	2.26	0.43
9:A:1900:C:OP2	9:A:1917:G:N2	2.44	0.43
10:K:158:SER:O	10:K:161:VAL:HG12	2.18	0.43
39:G:90:LEU:O	39:G:93:LEU:C	2.61	0.43
56:H:40:PRO:HA	56:H:45:THR:HG22	2.00	0.43
8:3:14:SER:OG	8:3:17:ASN:OD1	2.32	0.43
9:A:700:U:O2'	12:M:101:ARG:NH2	2.51	0.43
9:A:869:U:O2'	9:A:1387:A:N1	2.50	0.43
9:A:3037:C:O2	9:A:3104:A:O2'	2.32	0.43
27:Z:11:ILE:O	31:6:33:ARG:NH2	2.51	0.43
46:l:28:THR:O	46:l:32:THR:HG22	2.18	0.43
50:q:92:THR:O	50:q:92:THR:HG22	2.18	0.43
4:d:45:ILE:HA	4:d:62:VAL:HG13	2.00	0.43
5:B:19:G:N2	5:B:20:G:N3	2.66	0.43
6:j:15:MET:CG	6:j:34:LEU:HD21	2.48	0.43
9:A:2877:U:OP2	9:A:2878:A:O2'	2.27	0.43
28:1:75:ASP:N	28:1:79:LYS:O	2.45	0.43
29:2:45:GLN:HB3	29:2:47:LEU:HD21	2.00	0.43
55:I:732:LEU:HD22	55:I:784:VAL:HA	1.99	0.43
4:d:20:ASP:OD1	4:d:21:VAL:N	2.52	0.43
9:A:2093:G:O2'	9:A:2094:G:OP2	2.25	0.43
29:2:84:ASP:OD2	29:2:93:GLN:NE2	2.51	0.43
39:G:104:GLU:OE2	39:G:105:VAL:N	2.52	0.43
1:c:16:GLY:C	1:c:17:THR:HG1	2.21	0.43
9:A:1339:G:OP1	25:X:72:LYS:NZ	2.47	0.43
9:A:2044:U:OP2	10:K:222:ARG:NH1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:106:ILE:HD12	18:T:119:GLN:CD	2.43	0.43
37:a:975:G:O2'	37:a:976:A:N7	2.51	0.43
37:a:1133:G:OP1	46:l:70:HIS:ND1	2.44	0.43
42:g:30:ILE:HD13	42:g:71:THR:HG22	2.00	0.43
2:y:58:ILE:HG23	2:y:66:VAL:HG11	2.01	0.43
5:B:37:C:N3	5:B:50:C:O2'	2.40	0.43
14:P:2:SER:OG	14:P:3:ARG:N	2.50	0.43
37:a:908:G:N1	54:v:16:A:OP2	2.45	0.43
39:G:65:VAL:O	39:G:65:VAL:HG12	2.18	0.43
44:i:8:ALA:O	44:i:12:THR:HG23	2.19	0.43
53:u:57:VAL:O	53:u:61:VAL:HG23	2.18	0.43
4:d:44:PHE:O	4:d:62:VAL:HG13	2.10	0.43
9:A:81:A:N6	9:A:97:U:O4'	2.52	0.43
9:A:1182:C:O2'	55:I:776:HIS:O	2.36	0.43
9:A:1474:A:OP2	9:A:1486:G:N1	2.46	0.43
9:A:2356:G:HO2'	9:A:2357:A:P	2.39	0.43
13:O:44:ASN:OD1	13:O:45:MET:N	2.52	0.43
48:n:71:GLY:O	48:n:99:ARG:NH2	2.52	0.43
19:U:34:GLY:N	19:U:37:ASP:OD2	2.49	0.43
37:a:769:U:O2'	37:a:771:G:N7	2.36	0.43
4:d:58:VAL:O	4:d:59:PRO:C	2.61	0.43
6:j:106:ASN:OD1	6:j:106:ASN:N	2.52	0.43
8:3:6:ARG:NH2	9:A:1252:G:O6	2.48	0.43
9:A:1130:C:O2	18:T:27:ARG:NE	2.50	0.43
37:a:898:G:OP1	38:b:9:ARG:NH2	2.51	0.43
55:I:675:ILE:HD11	55:I:710:TRP:HB3	2.01	0.43
56:H:12:VAL:HG12	56:H:47:PRO:HG2	2.00	0.43
4:d:32:LYS:NZ	4:d:53:ASP:OD2	2.52	0.43
4:d:50:ALA:HB1	4:d:57:HIS:CE1	2.54	0.43
9:A:2914:A:OP1	21:J:9:ARG:NH2	2.50	0.43
40:e:70:TYR:OH	40:e:92:ARG:NH1	2.52	0.43
40:e:78:PRO:O	40:e:84:ASN:ND2	2.45	0.43
49:p:53:ARG:O	49:p:57:LEU:HD23	2.19	0.43
9:A:1624:U:HO2'	9:A:1625:G:C5'	2.29	0.42
9:A:1679:A:O2'	9:A:1680:A:OP2	2.30	0.42
9:A:2795:C:O3'	11:L:156:THR:HB	2.19	0.42
12:M:119:ALA:HB2	12:M:124:ILE:HD12	2.00	0.42
56:H:28:THR:O	56:H:30:THR:HG22	2.19	0.42
9:A:935:A:N3	9:A:1060:U:O2'	2.45	0.42
10:K:53:HIS:CE1	10:K:220:THR:HG23	2.54	0.42
16:R:22:ALA:HB2	16:R:110:MET:HE1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:a:1273:C:OP1	43:h:37:SER:OG	2.36	0.42
42:g:14:LEU:HD11	42:g:84:SER:HB2	2.01	0.42
48:n:5:GLN:HA	48:n:8:VAL:HG22	2.01	0.42
50:q:24:ASP:OD1	50:q:25:ALA:N	2.51	0.42
53:u:70:VAL:HG12	53:u:92:VAL:HG22	2.01	0.42
58:9:88:ALA:HB2	58:9:93:LEU:HD12	2.00	0.42
9:A:2753:G:N7	36:F:31:ARG:NH1	2.64	0.42
9:A:2968:G:N2	14:P:144:GLN:OE1	2.52	0.42
12:M:135:THR:O	12:M:135:THR:HG23	2.18	0.42
20:V:134:ARG:NH2	20:V:146:GLU:OE2	2.48	0.42
43:h:130:GLY:C	43:h:131:LEU:HD12	2.44	0.42
46:l:66:GLU:HB3	58:9:99:ALA:HB2	2.00	0.42
3:E:572:U:O2	3:E:572:U:O2'	2.37	0.42
5:B:66:C:N4	5:B:107:A:OP2	2.50	0.42
9:A:2230:C:O2'	9:A:3044:A:N3	2.52	0.42
37:a:499:C:OP2	48:n:47:SER:OG	2.29	0.42
55:I:757:ASP:O	55:I:759:VAL:N	2.47	0.42
6:j:84:ILE:O	6:j:93:ARG:NH2	2.44	0.42
9:A:292:G:N2	9:A:343:U:O2	2.52	0.42
9:A:829:U:OP2	49:p:88:ARG:NH1	2.48	0.42
29:2:145:THR:O	29:2:162:ILE:HD11	2.19	0.42
37:a:1199:C:C2	37:a:1200:A:N7	2.87	0.42
53:u:209:SER:O	53:u:213:LEU:HD23	2.19	0.42
3:E:502:G:N2	9:A:2477:G:N2	2.67	0.42
9:A:582:G:N3	26:Y:68:ASN:ND2	2.63	0.42
56:H:13:VAL:HG13	56:H:22:GLN:OE1	2.20	0.42
58:9:17:VAL:O	58:9:21:ALA:HB3	2.20	0.42
2:y:13:PHE:CE2	2:y:27:ARG:HG2	2.54	0.42
9:A:1164:A:O2'	16:R:6:LYS:NZ	2.52	0.42
9:A:1165:G:O2'	9:A:1228:A:N6	2.45	0.42
9:A:1485:C:H2'	9:A:1486:G:O4'	2.20	0.42
9:A:1856:C:O2	9:A:2922:U:O2'	2.37	0.42
9:A:2019:A:OP2	9:A:2031:G:N1	2.44	0.42
10:K:137:PRO:O	10:K:140:THR:OG1	2.33	0.42
41:f:59:THR:HG21	41:f:75:TYR:OH	2.19	0.42
46:l:36:VAL:HG22	46:l:76:ILE:HG22	2.00	0.42
46:l:51:VAL:HG13	58:9:81:ARG:HB2	2.01	0.42
55:I:749:SER:O	55:I:749:SER:OG	2.30	0.42
57:o:29:VAL:HG23	57:o:29:VAL:O	2.20	0.42
58:9:80:SER:O	58:9:84:VAL:HG23	2.20	0.42
9:A:2332:U:N3	9:A:2333:G:O6	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:124:ASP:OD1	10:K:125:ILE:N	2.53	0.42
37:a:620:A:N3	44:i:109:SER:OG	2.48	0.42
37:a:1168:G:H21	58:9:100:SER:CB	2.33	0.42
37:a:1287:G:HO2'	37:a:1288:A:H8	1.66	0.42
2:y:39:LEU:O	2:y:41:SER:N	2.53	0.42
19:U:71:ARG:NH1	19:U:122:LEU:O	2.48	0.42
25:X:53:ASP:OD2	25:X:54:ASP:N	2.51	0.42
29:2:53:ASP:OD1	29:2:54:PHE:N	2.53	0.42
41:f:139:VAL:HG11	41:f:165:THR:HG21	2.01	0.42
46:l:6:ILE:CD1	46:l:76:ILE:HD11	2.47	0.42
48:n:33:VAL:HG13	48:n:79:MET:HE1	2.01	0.42
9:A:2843:C:O2'	11:L:164:THR:OG1	2.38	0.41
10:K:101:GLU:OE2	10:K:103:ARG:NH2	2.53	0.41
12:M:50:HIS:O	12:M:50:HIS:ND1	2.52	0.41
17:S:118:LEU:HD23	17:S:119:ASN:N	2.35	0.41
28:1:10:LEU:HD23	28:1:80:PRO:HG3	2.02	0.41
37:a:481:G:OP1	48:n:114:ARG:NH2	2.46	0.41
39:G:120:ALA:HB1	39:G:189:ALA:HB2	2.01	0.41
40:e:52:GLU:CG	40:e:190:LEU:HD11	2.49	0.41
40:e:104:ARG:O	40:e:105:THR:HG23	2.20	0.41
53:u:162:TRP:HZ3	53:u:200:ILE:HD13	1.84	0.41
55:I:668:THR:HG22	55:I:718:PHE:HE1	1.69	0.41
57:o:27:LEU:HD23	57:o:28:GLY:N	2.35	0.41
9:A:24:G:O2'	9:A:25:A:OP2	2.34	0.41
9:A:1212:U:H3'	9:A:1213:A:H5''	2.02	0.41
9:A:2243:C:O2'	24:W:28:ARG:NH2	2.51	0.41
33:8:11:ALA:O	33:8:15:SER:OG	2.35	0.41
37:a:40:C:O2'	48:n:114:ARG:NH2	2.52	0.41
37:a:792:G:OP1	37:a:884:G:N2	2.49	0.41
37:a:872:G:OP2	38:b:10:LYS:NZ	2.53	0.41
37:a:883:A:O2'	37:a:1497:A:OP1	2.22	0.41
37:a:1057:G:N2	37:a:1060:A:OP2	2.49	0.41
42:g:30:ILE:HG22	42:g:36:THR:HB	2.01	0.41
50:q:13:ILE:HG23	50:q:14:ARG:H	1.85	0.41
7:N:78:PRO:O	7:N:81:THR:HG22	2.20	0.41
9:A:926:U:H2'	20:V:24:ARG:HA	2.02	0.41
9:A:1116:C:O2	32:7:32:ARG:NH1	2.52	0.41
9:A:1875:U:OP1	11:L:146:ARG:N	2.53	0.41
37:a:874:A:O2'	37:a:1398:G:O2'	2.32	0.41
3:E:555:U:N3	3:E:558:A:OP2	2.46	0.41
6:j:96:LEU:HD22	6:j:103:THR:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:54:THR:O	12:M:58:VAL:HG23	2.20	0.41
53:u:107:VAL:CG1	53:u:148:LEU:HD21	2.50	0.41
2:y:58:ILE:HG12	2:y:66:VAL:HG21	2.01	0.41
9:A:2371:G:O2'	9:A:2372:U:O4'	2.26	0.41
22:D:40:VAL:HG22	22:D:49:VAL:HG12	2.02	0.41
37:a:721:G:OP1	49:p:2:ALA:N	2.53	0.41
37:a:1260:A:O2'	37:a:1263:C:N4	2.53	0.41
37:a:1386:C:N4	54:v:18:G:OP1	2.52	0.41
46:l:10:LEU:CD2	46:l:98:VAL:HG12	2.49	0.41
55:I:675:ILE:HG22	55:I:689:ARG:HA	2.02	0.41
1:c:11:LEU:HD13	1:c:26:ASN:CB	2.42	0.41
9:A:251:A:OP1	35:x:7:HIS:NE2	2.44	0.41
9:A:1179:U:O2'	9:A:1181:G:OP1	2.39	0.41
9:A:1716:A:N3	9:A:1797:C:O2'	2.43	0.41
29:2:11:LEU:HD12	29:2:67:LEU:CD1	2.46	0.41
37:a:675:A:OP2	47:m:64:SER:N	2.50	0.41
53:u:100:MET:HA	53:u:107:VAL:HG21	2.01	0.41
5:B:55:G:HO2'	5:B:56:C:H6	1.66	0.41
9:A:730:G:N1	20:V:77:VAL:HG11	2.36	0.41
10:K:158:SER:OG	10:K:159:ALA:N	2.53	0.41
37:a:543:A:O2'	37:a:546:G:O3'	2.38	0.41
39:G:124:SER:HB2	39:G:191:THR:HG22	2.03	0.41
50:q:49:ILE:HG22	50:q:49:ILE:O	2.21	0.41
53:u:15:HIS:HB3	53:u:43:LEU:HD11	2.02	0.41
9:A:2615:G:N2	9:A:2653:G:O4'	2.54	0.41
6:j:51:ASP:OD1	6:j:51:ASP:N	2.53	0.41
9:A:284:G:O6	15:Q:106:LYS:NZ	2.35	0.41
9:A:368:U:O2	9:A:434:G:C6	2.73	0.41
9:A:845:C:OP1	9:A:1992:U:O2'	2.23	0.41
9:A:1164:A:O3'	16:R:6:LYS:NZ	2.54	0.41
9:A:3071:A:OP2	9:A:3087:G:N1	2.48	0.41
16:R:17:PHE:CD1	16:R:23:THR:HG21	2.52	0.41
17:S:106:GLN:HE22	17:S:110:ILE:HD11	1.86	0.41
21:J:36:THR:OG1	21:J:37:THR:N	2.54	0.41
36:F:14:CYS:SG	36:F:32:HIS:ND1	2.94	0.41
37:a:1200:A:OP1	58:9:59:ARG:NH2	2.53	0.41
37:a:1230:C:O2'	45:k:95:GLN:NE2	2.54	0.41
40:e:139:ASP:OD1	40:e:174:ARG:NE	2.53	0.41
45:k:68:ILE:HD11	45:k:96:ALA:HA	2.02	0.41
46:l:29:VAL:HG21	46:l:36:VAL:HG21	2.02	0.41
49:p:4:THR:HG22	49:p:7:GLN:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:u:147:SER:OG	53:u:148:LEU:N	2.54	0.41
4:d:15:LEU:HD23	4:d:15:LEU:C	2.45	0.41
5:B:30:G:H21	5:B:59:A:N6	2.18	0.41
9:A:671:G:O2'	9:A:2243:C:OP1	2.38	0.41
23:C:13:ARG:NH1	23:C:80:ILE:O	2.47	0.41
55:I:745:VAL:CG1	55:I:765:THR:HG23	2.50	0.41
13:O:173:GLY:O	13:O:177:LEU:HD23	2.21	0.40
23:C:73:PHE:HB3	23:C:80:ILE:HD11	2.03	0.40
40:e:24:GLN:OE1	40:e:24:GLN:N	2.55	0.40
48:n:35:THR:N	48:n:54:ARG:O	2.52	0.40
3:E:565:U:HO2'	3:E:566:C:P	2.44	0.40
4:d:33:THR:CG2	4:d:51:VAL:HG12	2.51	0.40
9:A:1186:G:H21	9:A:1214:A:C4'	2.34	0.40
9:A:1541:G:OP2	9:A:1629:G:N2	2.32	0.40
2:y:63:ILE:O	2:y:67:VAL:HG23	2.21	0.40
3:E:542:A:H3'	3:E:543:G:H4'	2.04	0.40
9:A:81:A:N1	9:A:96:G:O2'	2.46	0.40
9:A:1225:G:OP2	16:R:53:LYS:NZ	2.54	0.40
9:A:1319:A:OP1	12:M:153:LYS:NZ	2.43	0.40
27:Z:17:SER:N	27:Z:20:SER:OG	2.54	0.40
37:a:452:A:O2'	37:a:453:G:OP1	2.36	0.40
41:f:159:ILE:HD12	41:f:159:ILE:H	1.86	0.40
9:A:287:A:N6	9:A:299:G:N3	2.69	0.40
9:A:2328:G:H2'	9:A:2329:G:O4'	2.21	0.40
9:A:2429:A:OP1	10:K:68:ARG:NH2	2.54	0.40
9:A:2619:C:H2'	9:A:2620:G:O4'	2.21	0.40
17:S:81:LEU:HD21	17:S:139:ILE:HG21	2.03	0.40
29:2:170:LEU:HD22	29:2:172:SER:HB2	2.02	0.40
37:a:1476:A:P	48:n:44:LYS:HD2	2.61	0.40
53:u:130:THR:OG1	53:u:131:LYS:N	2.55	0.40
56:H:30:THR:OG1	56:H:31:SER:N	2.55	0.40
7:N:56:ARG:HE	55:I:729:ARG:HB3	1.87	0.40
9:A:406:A:N6	9:A:420:G:O2'	2.50	0.40
9:A:2981:A:N1	14:P:68:LEU:HD13	2.37	0.40
9:A:3032:G:H5''	11:L:63:ILE:HG23	2.04	0.40
11:L:151:ILE:HD12	11:L:166:MET:HE3	2.03	0.40
37:a:438:U:O2'	37:a:439:U:O5'	2.40	0.40
37:a:686:A:H2	47:m:50:VAL:HG21	1.87	0.40
39:G:120:ALA:CB	39:G:189:ALA:HB2	2.51	0.40
41:f:38:GLU:OE1	41:f:38:GLU:N	2.54	0.40
50:q:13:ILE:HG23	50:q:14:ARG:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	c	47/53 (89%)	36 (77%)	11 (23%)	0	100	100
2	y	74/77 (96%)	63 (85%)	11 (15%)	0	100	100
4	d	80/82 (98%)	73 (91%)	6 (8%)	1 (1%)	9	18
6	j	114/116 (98%)	94 (82%)	18 (16%)	2 (2%)	6	13
7	N	134/136 (98%)	127 (95%)	7 (5%)	0	100	100
8	3	21/23 (91%)	21 (100%)	0	0	100	100
10	K	273/275 (99%)	259 (95%)	14 (5%)	0	100	100
11	L	212/214 (99%)	194 (92%)	18 (8%)	0	100	100
12	M	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
13	O	180/182 (99%)	167 (93%)	13 (7%)	0	100	100
14	P	174/176 (99%)	164 (94%)	10 (6%)	0	100	100
15	Q	149/151 (99%)	132 (89%)	17 (11%)	0	100	100
16	R	124/126 (98%)	108 (87%)	16 (13%)	0	100	100
17	S	131/133 (98%)	104 (79%)	27 (21%)	0	100	100
18	T	144/146 (99%)	138 (96%)	6 (4%)	0	100	100
19	U	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
20	V	143/145 (99%)	133 (93%)	10 (7%)	0	100	100
21	J	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
22	D	124/126 (98%)	123 (99%)	1 (1%)	0	100	100
23	C	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
24	W	122/124 (98%)	120 (98%)	2 (2%)	0	100	100
25	X	98/100 (98%)	98 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Y	112/114 (98%)	106 (95%)	6 (5%)	0	100	100
27	Z	95/97 (98%)	88 (93%)	7 (7%)	0	100	100
28	1	93/105 (89%)	87 (94%)	6 (6%)	0	100	100
29	2	178/192 (93%)	164 (92%)	14 (8%)	0	100	100
30	4	77/79 (98%)	75 (97%)	2 (3%)	0	100	100
31	6	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
32	7	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
33	8	52/54 (96%)	48 (92%)	4 (8%)	0	100	100
34	0	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
35	x	61/63 (97%)	61 (100%)	0	0	100	100
36	F	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
38	b	30/32 (94%)	30 (100%)	0	0	100	100
39	G	206/208 (99%)	179 (87%)	26 (13%)	1 (0%)	24	43
40	e	198/200 (99%)	177 (89%)	21 (11%)	0	100	100
41	f	178/180 (99%)	165 (93%)	13 (7%)	0	100	100
42	g	94/96 (98%)	87 (93%)	7 (7%)	0	100	100
43	h	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
44	i	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
45	k	124/126 (98%)	111 (90%)	13 (10%)	0	100	100
46	l	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
47	m	113/115 (98%)	101 (89%)	12 (11%)	0	100	100
48	n	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
49	p	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
50	q	111/113 (98%)	95 (86%)	16 (14%)	0	100	100
51	r	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
52	t	83/85 (98%)	83 (100%)	0	0	100	100
53	u	226/228 (99%)	213 (94%)	13 (6%)	0	100	100
55	I	148/797 (19%)	112 (76%)	36 (24%)	0	100	100
56	H	71/82 (87%)	63 (89%)	8 (11%)	0	100	100
57	o	67/84 (80%)	61 (91%)	6 (9%)	0	100	100
58	9	98/100 (98%)	90 (92%)	8 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	6188/6992 (88%)	5721 (92%)	463 (8%)	4 (0%)	49 71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	d	37	ARG
6	j	83	GLU
39	G	126	ARG
6	j	82	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
1	c	46/49 (94%)	42 (91%)	4 (9%)	9 18
2	y	63/64 (98%)	61 (97%)	2 (3%)	34 58
4	d	73/73 (100%)	70 (96%)	3 (4%)	27 49
6	j	99/99 (100%)	98 (99%)	1 (1%)	68 81
7	N	114/114 (100%)	114 (100%)	0	100 100
8	3	18/18 (100%)	18 (100%)	0	100 100
10	K	215/215 (100%)	215 (100%)	0	100 100
11	L	160/160 (100%)	160 (100%)	0	100 100
12	M	169/169 (100%)	169 (100%)	0	100 100
13	O	151/151 (100%)	151 (100%)	0	100 100
14	P	148/148 (100%)	148 (100%)	0	100 100
15	Q	90/116 (78%)	90 (100%)	0	100 100
16	R	89/89 (100%)	89 (100%)	0	100 100
17	S	102/102 (100%)	102 (100%)	0	100 100
18	T	119/119 (100%)	119 (100%)	0	100 100
19	U	100/100 (100%)	100 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	V	112/112 (100%)	112 (100%)	0	100	100
21	J	97/97 (100%)	97 (100%)	0	100	100
22	D	93/93 (100%)	93 (100%)	0	100	100
23	C	100/100 (100%)	100 (100%)	0	100	100
24	W	97/97 (100%)	97 (100%)	0	100	100
25	X	81/81 (100%)	81 (100%)	0	100	100
26	Y	90/90 (100%)	90 (100%)	0	100	100
27	Z	83/83 (100%)	83 (100%)	0	100	100
28	1	81/86 (94%)	81 (100%)	0	100	100
29	2	148/155 (96%)	148 (100%)	0	100	100
30	4	58/58 (100%)	58 (100%)	0	100	100
31	6	58/58 (100%)	58 (100%)	0	100	100
32	7	52/52 (100%)	52 (100%)	0	100	100
33	8	43/43 (100%)	43 (100%)	0	100	100
34	0	35/35 (100%)	35 (100%)	0	100	100
35	x	53/53 (100%)	53 (100%)	0	100	100
36	F	35/35 (100%)	35 (100%)	0	100	100
38	b	30/30 (100%)	30 (100%)	0	100	100
39	G	170/170 (100%)	168 (99%)	2 (1%)	63	78
40	e	175/175 (100%)	175 (100%)	0	100	100
41	f	127/127 (100%)	127 (100%)	0	100	100
42	g	85/85 (100%)	85 (100%)	0	100	100
43	h	131/131 (100%)	131 (100%)	0	100	100
44	i	107/107 (100%)	107 (100%)	0	100	100
45	k	102/102 (100%)	102 (100%)	0	100	100
46	l	89/89 (100%)	89 (100%)	0	100	100
47	m	89/89 (100%)	89 (100%)	0	100	100
48	n	103/103 (100%)	103 (100%)	0	100	100
49	p	76/76 (100%)	76 (100%)	0	100	100
50	q	92/92 (100%)	92 (100%)	0	100	100
51	r	80/80 (100%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	t	69/69 (100%)	69 (100%)	0	100	100
53	u	191/191 (100%)	191 (100%)	0	100	100
55	I	128/653 (20%)	128 (100%)	0	100	100
56	H	64/70 (91%)	64 (100%)	0	100	100
57	o	58/70 (83%)	58 (100%)	0	100	100
58	9	85/85 (100%)	85 (100%)	0	100	100
All	All	5123/5708 (90%)	5111 (100%)	12 (0%)	85	95

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	c	9	VAL
1	c	10	LYS
1	c	43	LEU
1	c	52	GLU
2	y	16	SER
2	y	17	VAL
4	d	36	ARG
4	d	55	ARG
4	d	56	LYS
6	j	83	GLU
39	G	123	LEU
39	G	126	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	c	26	ASN
1	c	29	ASN
2	y	15	ASN
4	d	47	HIS
4	d	52	HIS
4	d	57	HIS
4	d	69	HIS
10	K	38	HIS
13	O	62	ASN
17	S	45	ASN
18	T	111	HIS
18	T	135	GLN

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Mol	Chain	Res	Type
21	J	17	GLN
24	W	39	GLN
27	Z	63	GLN
29	2	76	GLN
29	2	169	ASN
31	6	31	ASN
32	7	8	GLN
35	x	25	GLN
35	x	28	ASN
39	G	125	ASN
39	G	143	GLN
43	h	86	GLN
43	h	153	HIS
45	k	86	HIS
46	l	56	HIS
47	m	84	GLN
48	n	112	GLN
53	u	19	GLN
55	I	701	GLN
56	H	15	GLN
57	o	22	ASN
57	o	54	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	E	76/77 (98%)	40 (52%)	4 (5%)
37	a	1510/1511 (99%)	319 (21%)	0
5	B	117/118 (99%)	27 (23%)	2 (1%)
54	v	17/20 (85%)	10 (58%)	0
9	A	3118/3119 (99%)	632 (20%)	15 (0%)
All	All	4838/4845 (99%)	1028 (21%)	21 (0%)

All (1028) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	E	502	G
3	E	503	C
3	E	504	G
3	E	505	G
3	E	508	U

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Mol	Chain	Res	Type
3	E	514	A
3	E	515	G
3	E	516	C
3	E	518	U
3	E	518(A)	C
3	E	518(B)	G
3	E	519	G
3	E	520	U
3	E	521	A
3	E	522	G
3	E	534	C
3	E	535	A
3	E	537	A
3	E	538	A
3	E	542	A
3	E	543	G
3	E	548	C
3	E	549	G
3	E	554	U
3	E	555	U
3	E	557	G
3	E	558	A
3	E	559	A
3	E	563	U
3	E	564	G
3	E	566	C
3	E	567	C
3	E	568	C
3	E	569	C
3	E	570	G
3	E	571	C
3	E	572	U
3	E	573	A
3	E	574	C
3	E	576	A
5	B	3	U
5	B	4	A
5	B	5	C
5	B	6	G
5	B	12	C
5	B	13	C
5	B	20	G

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Mol	Chain	Res	Type
5	B	22	A
5	B	26	A
5	B	31	C
5	B	35	G
5	B	36	U
5	B	42	C
5	B	43	C
5	B	54	A
5	B	56	C
5	B	57	U
5	B	58	A
5	B	66	C
5	B	67	A
5	B	74	A
5	B	87	U
5	B	88	C
5	B	90	G
5	B	107	A
5	B	115	A
5	B	116	C
9	A	7	U
9	A	12	G
9	A	20	G
9	A	31	U
9	A	32	G
9	A	36	C
9	A	55	G
9	A	59	G
9	A	61	G
9	A	68	A
9	A	71	A
9	A	72	G
9	A	82	G
9	A	89	A
9	A	94	G
9	A	99	G
9	A	107	G
9	A	115	A
9	A	116	A
9	A	117	U
9	A	125	C
9	A	128	G

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Mol	Chain	Res	Type
9	A	136	U
9	A	145	G
9	A	153	G
9	A	164	A
9	A	174	G
9	A	175	G
9	A	180	A
9	A	186	G
9	A	195	A
9	A	198	A
9	A	212	A
9	A	214	G
9	A	215	A
9	A	220	A
9	A	221	A
9	A	224	C
9	A	227	A
9	A	229	U
9	A	230	G
9	A	233	A
9	A	248	G
9	A	268	G
9	A	275	C
9	A	285	U
9	A	286	G
9	A	287	A
9	A	288	U
9	A	291	C
9	A	292	G
9	A	297	G
9	A	298	G
9	A	299	G
9	A	300	G
9	A	301	U
9	A	302	U
9	A	303	G
9	A	304	U
9	A	305	G
9	A	313	G
9	A	314	G
9	A	315	U
9	A	317	G

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Mol	Chain	Res	Type
9	A	318	U
9	A	319	G
9	A	324	C
9	A	329	U
9	A	330	U
9	A	331	U
9	A	336	C
9	A	337	U
9	A	338	C
9	A	340	A
9	A	342	C
9	A	344	G
9	A	345	G
9	A	353	G
9	A	354	C
9	A	357	U
9	A	361	A
9	A	363	A
9	A	366	G
9	A	370	U
9	A	376	G
9	A	384	G
9	A	393	U
9	A	399	G
9	A	412	A
9	A	413	G
9	A	414	A
9	A	428	A
9	A	434	G
9	A	437	G
9	A	438	U
9	A	444	U
9	A	445	U
9	A	446	G
9	A	447	A
9	A	452	G
9	A	454	U
9	A	460	G
9	A	474	G
9	A	489	A
9	A	490	A
9	A	493	U

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Mol	Chain	Res	Type
9	A	494	G
9	A	498	G
9	A	512	G
9	A	523	U
9	A	536	U
9	A	539	C
9	A	543	U
9	A	544	U
9	A	566	A
9	A	567	A
9	A	568	A
9	A	569	G
9	A	581	G
9	A	583	G
9	A	585	G
9	A	588	A
9	A	589	A
9	A	591	G
9	A	592	A
9	A	594	U
9	A	595	A
9	A	596	C
9	A	605	G
9	A	614	C
9	A	617	U
9	A	618	C
9	A	619	C
9	A	620	G
9	A	635	G
9	A	636	U
9	A	637	G
9	A	639	C
9	A	640	G
9	A	642	G
9	A	644	G
9	A	647	G
9	A	655	G
9	A	665	G
9	A	667	A
9	A	675	G
9	A	679	G
9	A	684	G

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Mol	Chain	Res	Type
9	A	685	G
9	A	696	A
9	A	706	G
9	A	707	G
9	A	708	G
9	A	709	U
9	A	714	U
9	A	721	A
9	A	725	A
9	A	728	G
9	A	731	A
9	A	738	A
9	A	739	U
9	A	740	A
9	A	741	G
9	A	742	G
9	A	747	A
9	A	749	C
9	A	756	A
9	A	757	G
9	A	758	A
9	A	759	G
9	A	760	U
9	A	764	U
9	A	765	G
9	A	766	G
9	A	801	U
9	A	817	G
9	A	830	A
9	A	832	G
9	A	838	G
9	A	839	U
9	A	845	C
9	A	862	U
9	A	868	C
9	A	872	G
9	A	879	A
9	A	880	G
9	A	890	G
9	A	891	G
9	A	897	A
9	A	899	G

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Mol	Chain	Res	Type
9	A	900	G
9	A	915	U
9	A	920	G
9	A	927	C
9	A	942	U
9	A	971	G
9	A	974	G
9	A	981	U
9	A	982	A
9	A	985	G
9	A	990	G
9	A	994	A
9	A	996	G
9	A	997	G
9	A	1001	C
9	A	1002	C
9	A	1003	A
9	A	1004	C
9	A	1007	G
9	A	1008	G
9	A	1011	A
9	A	1014	G
9	A	1022	C
9	A	1025	A
9	A	1030	C
9	A	1047	A
9	A	1049	G
9	A	1058	A
9	A	1063	G
9	A	1076	A
9	A	1078	G
9	A	1085	G
9	A	1092	G
9	A	1101	A
9	A	1103	C
9	A	1107	G
9	A	1108	A
9	A	1114	G
9	A	1131	G
9	A	1135	G
9	A	1140	G
9	A	1141	U

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Mol	Chain	Res	Type
9	A	1143	G
9	A	1144	A
9	A	1151	U
9	A	1157	G
9	A	1163	A
9	A	1164	A
9	A	1175	A
9	A	1178	U
9	A	1180	G
9	A	1181	G
9	A	1184	U
9	A	1185	A
9	A	1186	G
9	A	1187	A
9	A	1188	A
9	A	1189	G
9	A	1190	C
9	A	1191	A
9	A	1193	C
9	A	1194	C
9	A	1197	C
9	A	1201	G
9	A	1202	A
9	A	1203	A
9	A	1205	G
9	A	1206	A
9	A	1207	G
9	A	1208	U
9	A	1209	G
9	A	1212	U
9	A	1213	A
9	A	1214	A
9	A	1215	U
9	A	1217	G
9	A	1219	U
9	A	1220	C
9	A	1226	U
9	A	1230	G
9	A	1238	G
9	A	1240	G
9	A	1246	A
9	A	1250	U

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Mol	Chain	Res	Type
9	A	1251	A
9	A	1253	C
9	A	1254	G
9	A	1260	C
9	A	1261	A
9	A	1267	A
9	A	1270	G
9	A	1292	U
9	A	1293	G
9	A	1332	G
9	A	1335	G
9	A	1344	A
9	A	1347	G
9	A	1353	G
9	A	1359	G
9	A	1368	A
9	A	1371	G
9	A	1380	A
9	A	1386	G
9	A	1387	A
9	A	1389	U
9	A	1409	C
9	A	1415	A
9	A	1416	A
9	A	1421	C
9	A	1428	U
9	A	1456	G
9	A	1465	C
9	A	1467	U
9	A	1480	A
9	A	1485	C
9	A	1493	A
9	A	1494	U
9	A	1501	C
9	A	1507	G
9	A	1510	A
9	A	1518	A
9	A	1521	C
9	A	1522	G
9	A	1529	U
9	A	1531	C
9	A	1533	U

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Mol	Chain	Res	Type
9	A	1534	C
9	A	1538	G
9	A	1540	U
9	A	1542	A
9	A	1543	A
9	A	1549	G
9	A	1550	G
9	A	1551	U
9	A	1552	A
9	A	1553	C
9	A	1554	U
9	A	1556	A
9	A	1557	C
9	A	1563	A
9	A	1564	A
9	A	1565	A
9	A	1566	A
9	A	1567	C
9	A	1571	C
9	A	1574	G
9	A	1587	G
9	A	1588	G
9	A	1589	G
9	A	1597	G
9	A	1598	U
9	A	1599	U
9	A	1600	G
9	A	1617	C
9	A	1623	U
9	A	1625	G
9	A	1629	G
9	A	1630	U
9	A	1632	G
9	A	1636	A
9	A	1639	G
9	A	1640	A
9	A	1641	U
9	A	1648	A
9	A	1649	C
9	A	1658	G
9	A	1676	G
9	A	1679	A

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Mol	Chain	Res	Type
9	A	1681	U
9	A	1688	G
9	A	1694	C
9	A	1703	G
9	A	1710	A
9	A	1711	G
9	A	1713	U
9	A	1714	A
9	A	1716	A
9	A	1717	U
9	A	1720	G
9	A	1724	G
9	A	1728	U
9	A	1731	A
9	A	1737	A
9	A	1754	G
9	A	1755	A
9	A	1756	G
9	A	1757	U
9	A	1758	G
9	A	1769	G
9	A	1786	G
9	A	1789	A
9	A	1798	U
9	A	1804	G
9	A	1813	C
9	A	1826	A
9	A	1828	A
9	A	1834	A
9	A	1843	C
9	A	1845	G
9	A	1848	A
9	A	1864	U
9	A	1866	C
9	A	1871	G
9	A	1872	A
9	A	1878	G
9	A	1892	G
9	A	1893	C
9	A	1895	A
9	A	1916	A
9	A	1946	U

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Mol	Chain	Res	Type
9	A	1947	U
9	A	1950	G
9	A	1955	A
9	A	1981	U
9	A	1990	A
9	A	2008	A
9	A	2017	C
9	A	2018	G
9	A	2024	G
9	A	2033	U
9	A	2046	A
9	A	2050	C
9	A	2065	A
9	A	2066	G
9	A	2075	G
9	A	2076	A
9	A	2086	U
9	A	2087	C
9	A	2088	C
9	A	2089	C
9	A	2090	U
9	A	2092	U
9	A	2093	G
9	A	2094	G
9	A	2095	G
9	A	2096	G
9	A	2104	G
9	A	2106	A
9	A	2107	G
9	A	2129	C
9	A	2130	G
9	A	2137	A
9	A	2138	C
9	A	2140	A
9	A	2141	U
9	A	2151	A
9	A	2153	G
9	A	2154	G
9	A	2160	A
9	A	2163	U
9	A	2179	U
9	A	2187	U

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Mol	Chain	Res	Type
9	A	2189	C
9	A	2191	C
9	A	2194	A
9	A	2195	U
9	A	2196	G
9	A	2215	U
9	A	2217	U
9	A	2221	A
9	A	2255	A
9	A	2256	G
9	A	2263	G
9	A	2267	C
9	A	2273	G
9	A	2278	A
9	A	2279	C
9	A	2280	G
9	A	2284	A
9	A	2285	G
9	A	2286	A
9	A	2303	A
9	A	2316	G
9	A	2317	G
9	A	2320	C
9	A	2323	G
9	A	2324	A
9	A	2328	G
9	A	2329	G
9	A	2331	U
9	A	2334	U
9	A	2335	G
9	A	2336	U
9	A	2337	A
9	A	2338	G
9	A	2339	G
9	A	2340	A
9	A	2341	U
9	A	2342	A
9	A	2343	G
9	A	2344	G
9	A	2346	G
9	A	2351	A
9	A	2353	U

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Mol	Chain	Res	Type
9	A	2354	G
9	A	2355	U
9	A	2357	A
9	A	2358	A
9	A	2360	C
9	A	2362	C
9	A	2365	A
9	A	2367	G
9	A	2368	C
9	A	2370	A
9	A	2371	G
9	A	2377	G
9	A	2379	G
9	A	2380	G
9	A	2381	A
9	A	2382	G
9	A	2383	U
9	A	2384	C
9	A	2385	G
9	A	2386	U
9	A	2387	U
9	A	2388	G
9	A	2392	A
9	A	2393	A
9	A	2394	A
9	A	2395	U
9	A	2396	A
9	A	2399	A
9	A	2402	C
9	A	2404	G
9	A	2407	C
9	A	2408	G
9	A	2418	U
9	A	2421	A
9	A	2427	G
9	A	2434	A
9	A	2436	A
9	A	2446	G
9	A	2447	G
9	A	2449	A
9	A	2462	G
9	A	2463	G

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Mol	Chain	Res	Type
9	A	2503	G
9	A	2507	C
9	A	2511	A
9	A	2512	A
9	A	2528	G
9	A	2529	A
9	A	2532	G
9	A	2544	U
9	A	2545	G
9	A	2549	G
9	A	2558	C
9	A	2559	A
9	A	2567	U
9	A	2569	G
9	A	2571	C
9	A	2574	C
9	A	2578	A
9	A	2596	G
9	A	2607	G
9	A	2609	A
9	A	2612	A
9	A	2647	U
9	A	2649	A
9	A	2653	G
9	A	2654	A
9	A	2655	U
9	A	2659	A
9	A	2665	C
9	A	2669	G
9	A	2672	A
9	A	2676	C
9	A	2693	A
9	A	2694	G
9	A	2699	C
9	A	2708	G
9	A	2715	U
9	A	2726	G
9	A	2729	G
9	A	2737	G
9	A	2742	A
9	A	2744	C
9	A	2749	G

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Mol	Chain	Res	Type
9	A	2753	G
9	A	2754	G
9	A	2759	G
9	A	2778	U
9	A	2785	A
9	A	2786	U
9	A	2788	A
9	A	2790	A
9	A	2791	G
9	A	2796	A
9	A	2797	C
9	A	2802	G
9	A	2806	G
9	A	2826	A
9	A	2827	G
9	A	2833	U
9	A	2837	U
9	A	2839	U
9	A	2845	G
9	A	2853	C
9	A	2854	A
9	A	2856	A
9	A	2862	G
9	A	2913	U
9	A	2926	A
9	A	2936	C
9	A	2938	G
9	A	2940	U
9	A	2942	G
9	A	2950	C
9	A	2957	A
9	A	2968	G
9	A	2972	A
9	A	2981	A
9	A	2982	A
9	A	2985	G
9	A	2989	A
9	A	2993	U
9	A	3002	A
9	A	3009	U
9	A	3014	A
9	A	3015	C

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Mol	Chain	Res	Type
9	A	3016	C
9	A	3021	A
9	A	3022	G
9	A	3023	G
9	A	3024	A
9	A	3029	U
9	A	3039	C
9	A	3042	A
9	A	3057	U
9	A	3082	U
9	A	3088	C
9	A	3093	A
9	A	3095	C
9	A	3098	G
9	A	3101	C
9	A	3104	A
9	A	3105	C
9	A	3106	C
9	A	3107	G
9	A	3112	A
9	A	3114	A
9	A	3115	A
37	a	10	G
37	a	11	G
37	a	12	A
37	a	13	G
37	a	36	A
37	a	43	G
37	a	45	G
37	a	48	G
37	a	52	U
37	a	55	A
37	a	75	A
37	a	82	U
37	a	87	G
37	a	92	A
37	a	93	C
37	a	115	A
37	a	117	C
37	a	118	A
37	a	123	G
37	a	126	G

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Mol	Chain	Res	Type
37	a	128	U
37	a	136	G
37	a	141	U
37	a	153	U
37	a	160	C
37	a	174	G
37	a	192	G
37	a	193	C
37	a	194	A
37	a	196	G
37	a	200	U
37	a	201	G
37	a	211	A
37	a	216	U
37	a	217	U
37	a	218	G
37	a	220	G
37	a	231	G
37	a	245	C
37	a	246	A
37	a	247	G
37	a	251	G
37	a	252	U
37	a	262	G
37	a	266	G
37	a	267	C
37	a	280	C
37	a	289	G
37	a	301	G
37	a	306	A
37	a	321	A
37	a	328	U
37	a	329	A
37	a	330	C
37	a	332	G
37	a	344	A
37	a	347	G
37	a	348	G
37	a	351	G
37	a	352	C
37	a	353	A
37	a	354	G

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Mol	Chain	Res	Type
37	a	367	U
37	a	372	C
37	a	373	A
37	a	389	A
37	a	392	C
37	a	396	G
37	a	397	A
37	a	398	C
37	a	406	G
37	a	411	A
37	a	412	U
37	a	413	G
37	a	414	A
37	a	421	U
37	a	422	C
37	a	423	G
37	a	426	U
37	a	427	U
37	a	428	G
37	a	429	U
37	a	430	A
37	a	433	C
37	a	438	U
37	a	439	U
37	a	452	A
37	a	453	G
37	a	456	C
37	a	457	A
37	a	458	A
37	a	459	G
37	a	465	G
37	a	466	U
37	a	469	G
37	a	470	U
37	a	471	G
37	a	472	C
37	a	475	A
37	a	477	G
37	a	480	G
37	a	488	C
37	a	489	A
37	a	490	A

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Mol	Chain	Res	Type
37	a	491	C
37	a	492	U
37	a	496	U
37	a	497	G
37	a	498	C
37	a	499	C
37	a	501	G
37	a	507	G
37	a	509	G
37	a	511	U
37	a	512	A
37	a	513	A
37	a	520	G
37	a	522	G
37	a	527	A
37	a	539	A
37	a	542	U
37	a	544	C
37	a	548	G
37	a	552	A
37	a	553	A
37	a	556	A
37	a	557	G
37	a	612	U
37	a	613	G
37	a	616	G
37	a	633	A
37	a	641	G
37	a	645	G
37	a	663	G
37	a	666	U
37	a	667	A
37	a	668	G
37	a	680	G
37	a	702	G
37	a	703	U
37	a	704	G
37	a	711	G
37	a	714	G
37	a	728	A
37	a	729	A
37	a	733	A

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Mol	Chain	Res	Type
37	a	735	G
37	a	739	A
37	a	761	A
37	a	765	G
37	a	772	A
37	a	773	U
37	a	774	A
37	a	779	G
37	a	789	G
37	a	793	U
37	a	794	A
37	a	795	A
37	a	796	A
37	a	797	C
37	a	808	A
37	a	812	G
37	a	818	U
37	a	822	U
37	a	823	U
37	a	824	C
37	a	825	C
37	a	826	U
37	a	827	U
37	a	828	G
37	a	835	G
37	a	840	G
37	a	841	U
37	a	854	A
37	a	858	A
37	a	869	G
37	a	871	A
37	a	884	G
37	a	895	A
37	a	896	A
37	a	898	G
37	a	908	G
37	a	909	G
37	a	914	C
37	a	916	C
37	a	917	A
37	a	924	G
37	a	940	A

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Mol	Chain	Res	Type
37	a	942	U
37	a	943	U
37	a	947	U
37	a	948	G
37	a	950	A
37	a	951	A
37	a	953	G
37	a	957	A
37	a	959	A
37	a	964	U
37	a	973	U
37	a	974	U
37	a	975	G
37	a	978	A
37	a	982	A
37	a	983	C
37	a	984	A
37	a	986	G
37	a	990	C
37	a	992	G
37	a	1000	U
37	a	1007	U
37	a	1008	C
37	a	1010	C
37	a	1012	U
37	a	1013	G
37	a	1014	U
37	a	1018	C
37	a	1020	G
37	a	1021	U
37	a	1022	G
37	a	1024	G
37	a	1025	C
37	a	1028	G
37	a	1030	G
37	a	1033	G
37	a	1034	C
37	a	1035	A
37	a	1036	U
37	a	1045	U
37	a	1046	C
37	a	1048	G

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Mol	Chain	Res	Type
37	a	1050	U
37	a	1065	U
37	a	1068	G
37	a	1074	G
37	a	1075	U
37	a	1081	A
37	a	1088	G
37	a	1100	U
37	a	1104	G
37	a	1105	U
37	a	1107	G
37	a	1110	A
37	a	1111	G
37	a	1113	A
37	a	1115	G
37	a	1116	U
37	a	1117	U
37	a	1118	A
37	a	1120	G
37	a	1138	A
37	a	1140	U
37	a	1149	C
37	a	1150	A
37	a	1151	A
37	a	1165	G
37	a	1177	A
37	a	1178	A
37	a	1193	U
37	a	1208	A
37	a	1217	A
37	a	1219	A
37	a	1229	A
37	a	1231	A
37	a	1238	U
37	a	1239	G
37	a	1241	G
37	a	1248	U
37	a	1249	G
37	a	1250	A
37	a	1251	G
37	a	1256	A
37	a	1261	A

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Mol	Chain	Res	Type
37	a	1266	U
37	a	1267	U
37	a	1269	A
37	a	1284	U
37	a	1287	G
37	a	1294	G
37	a	1299	C
37	a	1302	C
37	a	1320	G
37	a	1322	G
37	a	1328	A
37	a	1329	G
37	a	1335	G
37	a	1344	C
37	a	1345	A
37	a	1346	A
37	a	1351	G
37	a	1353	G
37	a	1357	A
37	a	1362	G
37	a	1364	U
37	a	1378	C
37	a	1380	C
37	a	1381	A
37	a	1405	G
37	a	1409	A
37	a	1423	U
37	a	1424	G
37	a	1425	G
37	a	1426	C
37	a	1429	A
37	a	1430	A
37	a	1434	U
37	a	1435	U
37	a	1436	G
37	a	1459	G
37	a	1478	G
37	a	1481	G
37	a	1483	A
37	a	1487	A
37	a	1488	G
37	a	1490	U

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Mol	Chain	Res	Type
37	a	1501	G
37	a	1503	A
37	a	1504	G
37	a	1513	G
37	a	1514	G
54	v	6	G
54	v	7	G
54	v	8	A
54	v	9	G
54	v	10	G
54	v	11	U
54	v	13	A
54	v	19	U
54	v	21	C
54	v	22	A

All (21) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	E	534	C
3	E	546	U
3	E	565	U
3	E	572	U
5	B	2	U
5	B	53	A
9	A	316	U
9	A	438	U
9	A	919	A
9	A	980	C
9	A	981	U
9	A	1102	G
9	A	1255	G
9	A	1291	G
9	A	1616	A
9	A	1730	U
9	A	2075	G
9	A	2094	G
9	A	2350	G
9	A	2356	G
9	A	2381	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

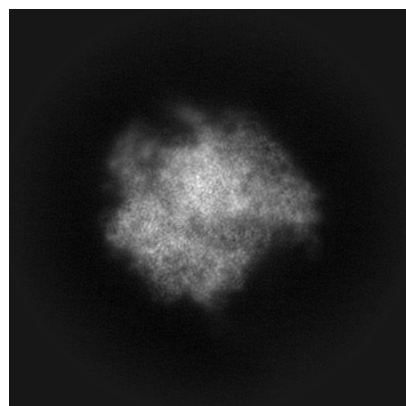
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29397. These allow visual inspection of the internal detail of the map and identification of artifacts.

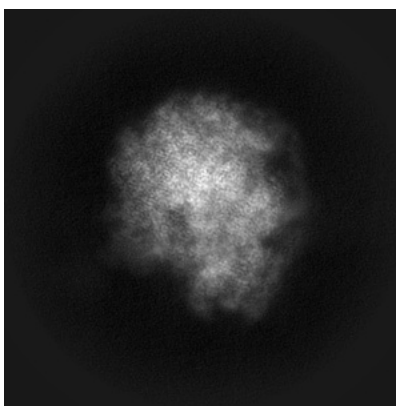
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

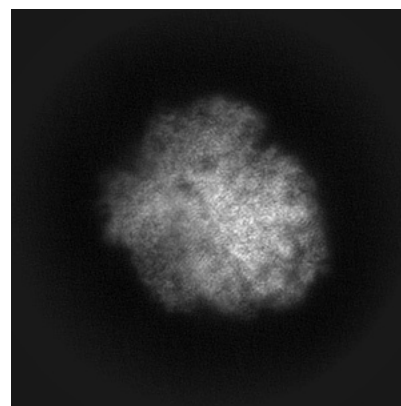
6.1.1 Primary map



X

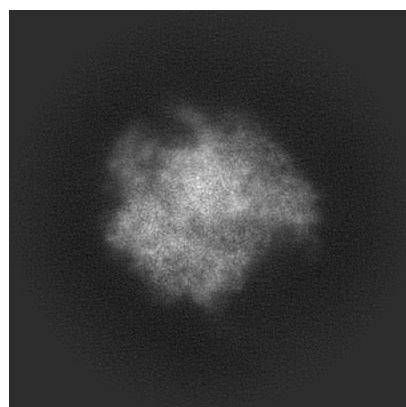


Y

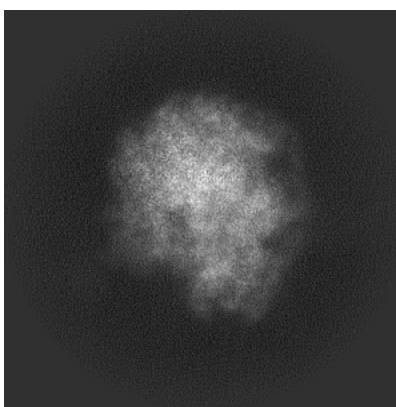


Z

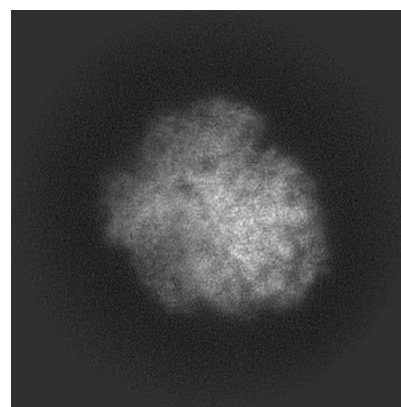
6.1.2 Raw map



X



Y

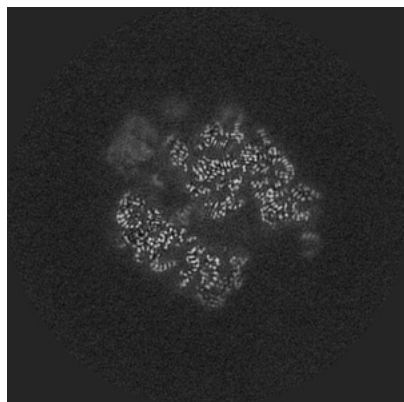


Z

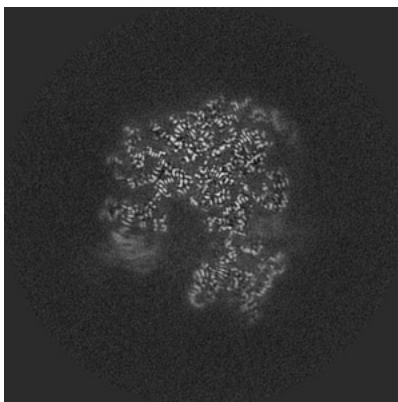
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

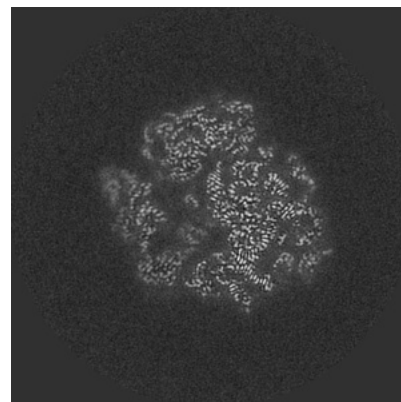
6.2.1 Primary map



X Index: 250

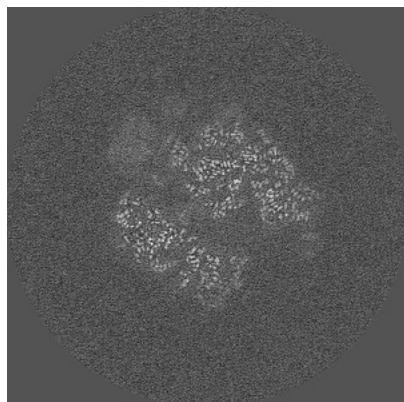


Y Index: 250

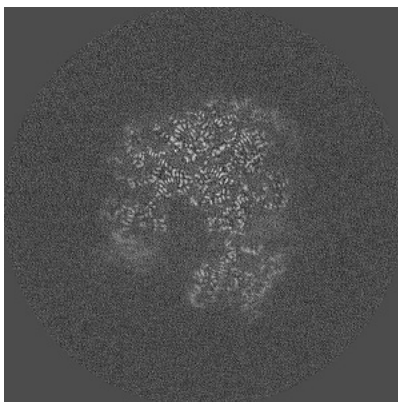


Z Index: 250

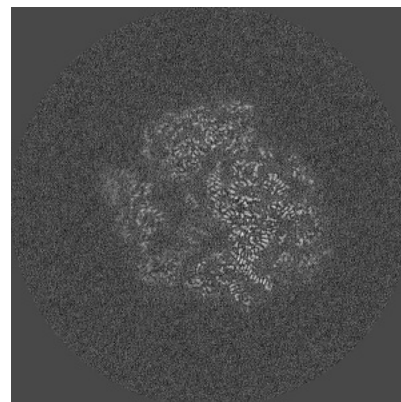
6.2.2 Raw map



X Index: 250



Y Index: 250

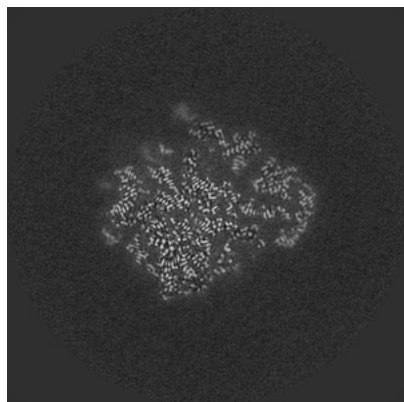


Z Index: 250

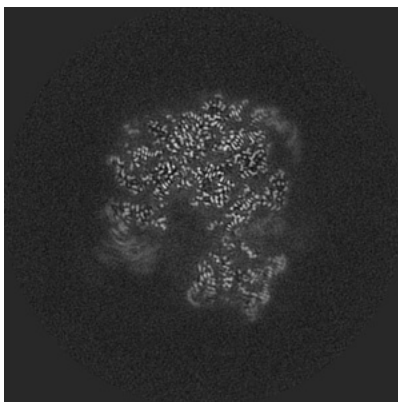
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

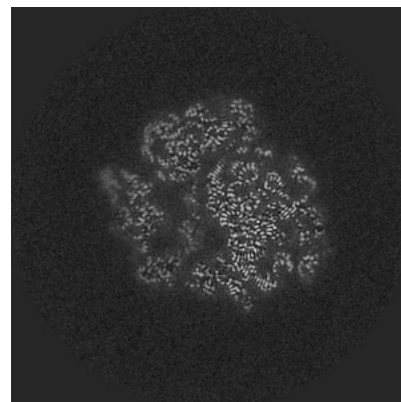
6.3.1 Primary map



X Index: 281

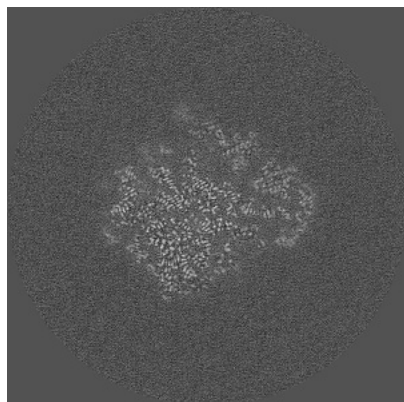


Y Index: 246

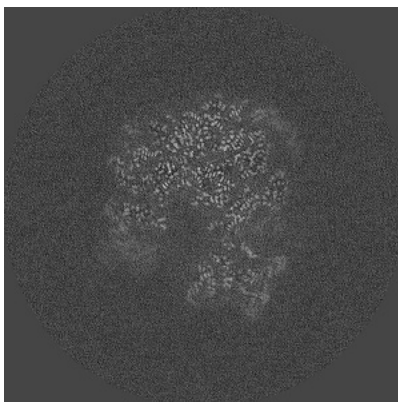


Z Index: 252

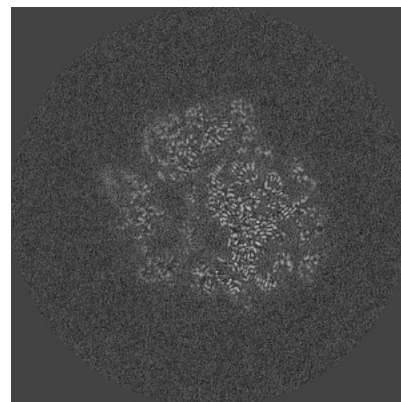
6.3.2 Raw map



X Index: 281



Y Index: 246



Z Index: 252

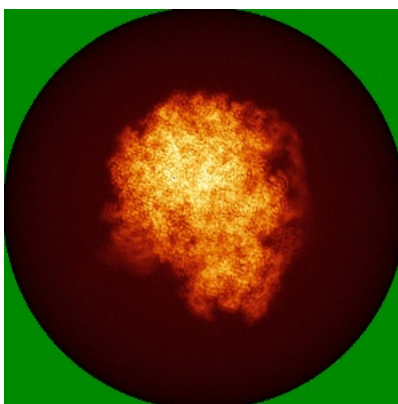
The images above show the largest variance slices of the map in three orthogonal directions.

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

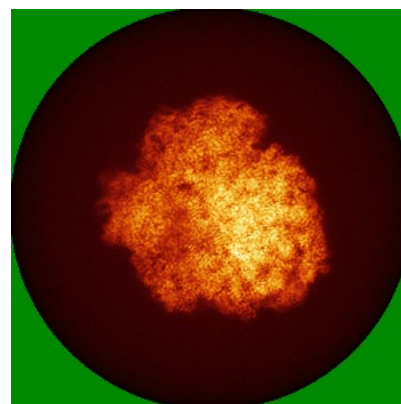
6.4.1 Primary map



X

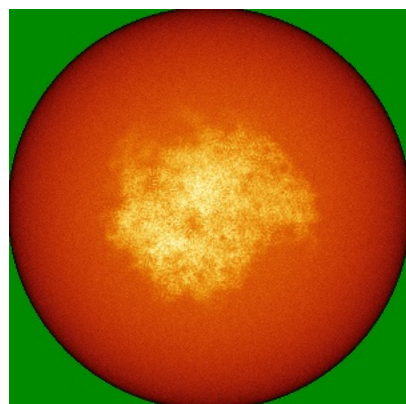


Y

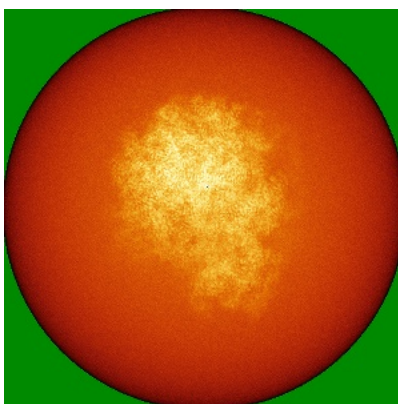


Z

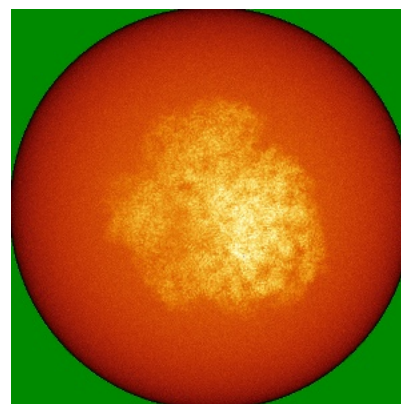
6.4.2 Raw map



X



Y

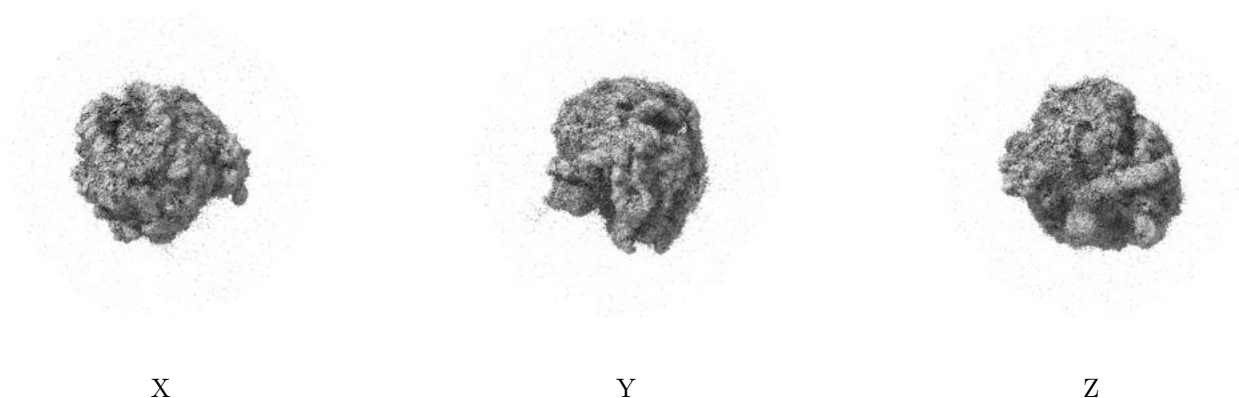


Z

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 0.003. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

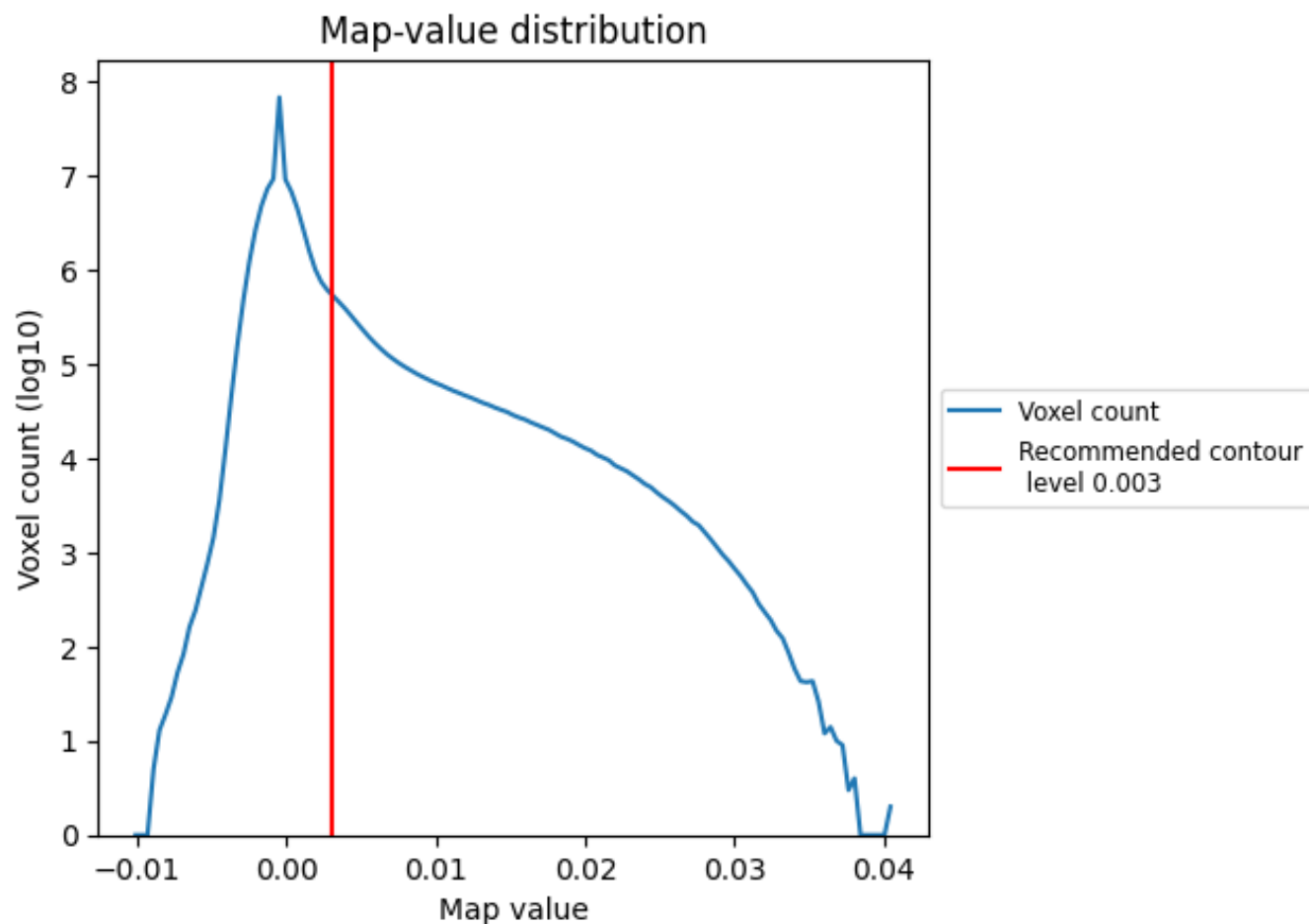
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

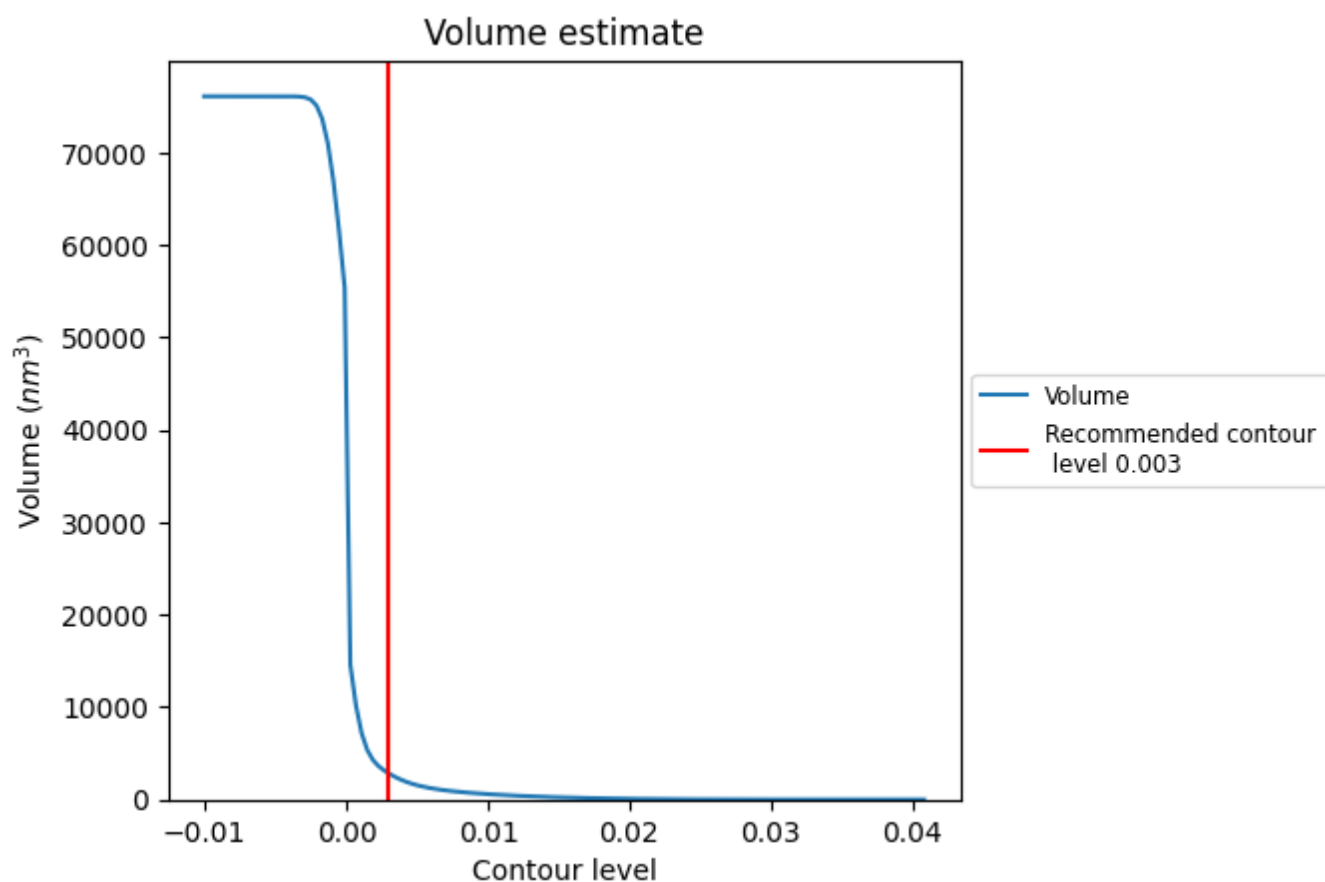
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

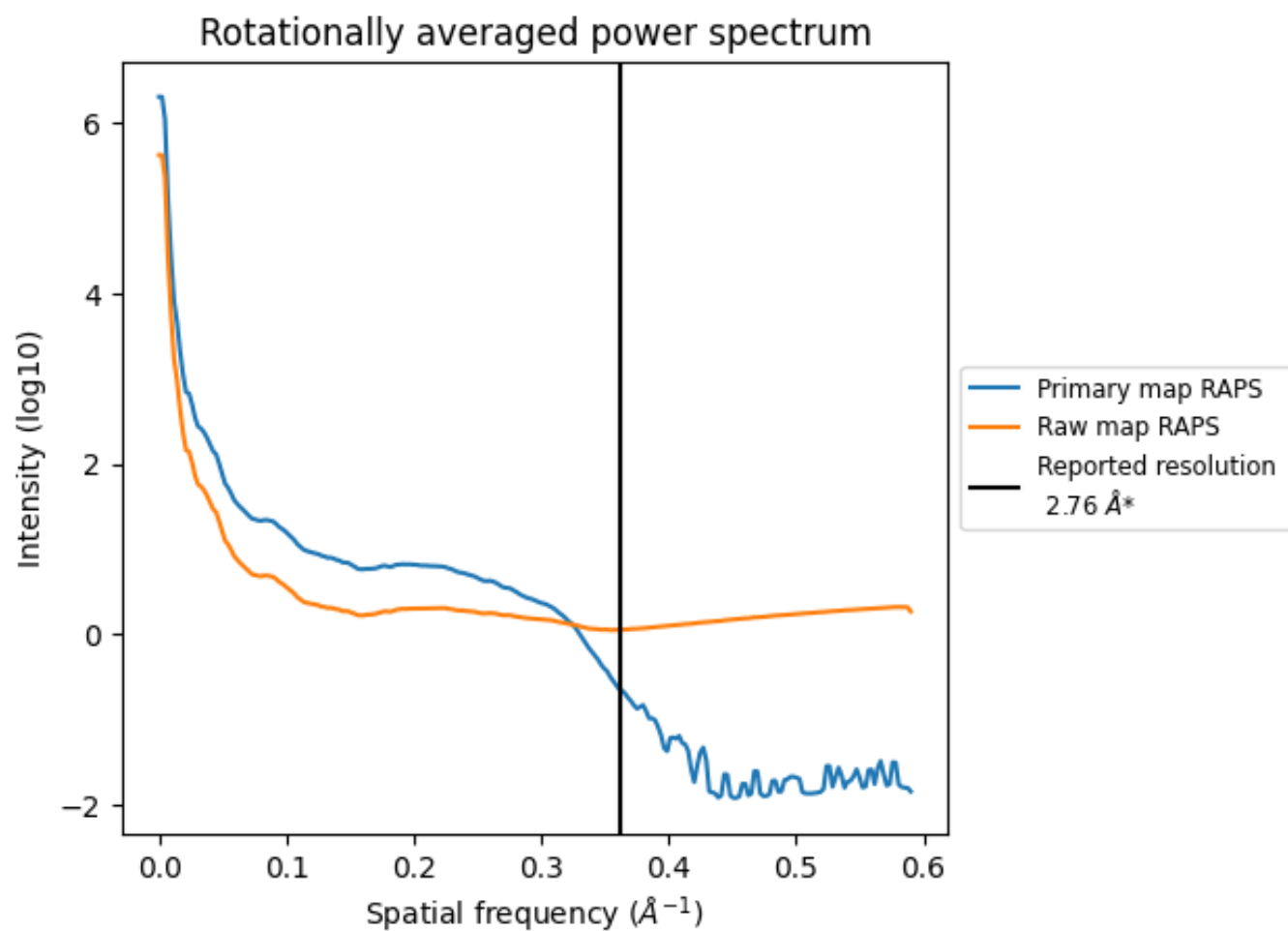
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2823 nm^3 ; this corresponds to an approximate mass of 2550 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 ⓘ

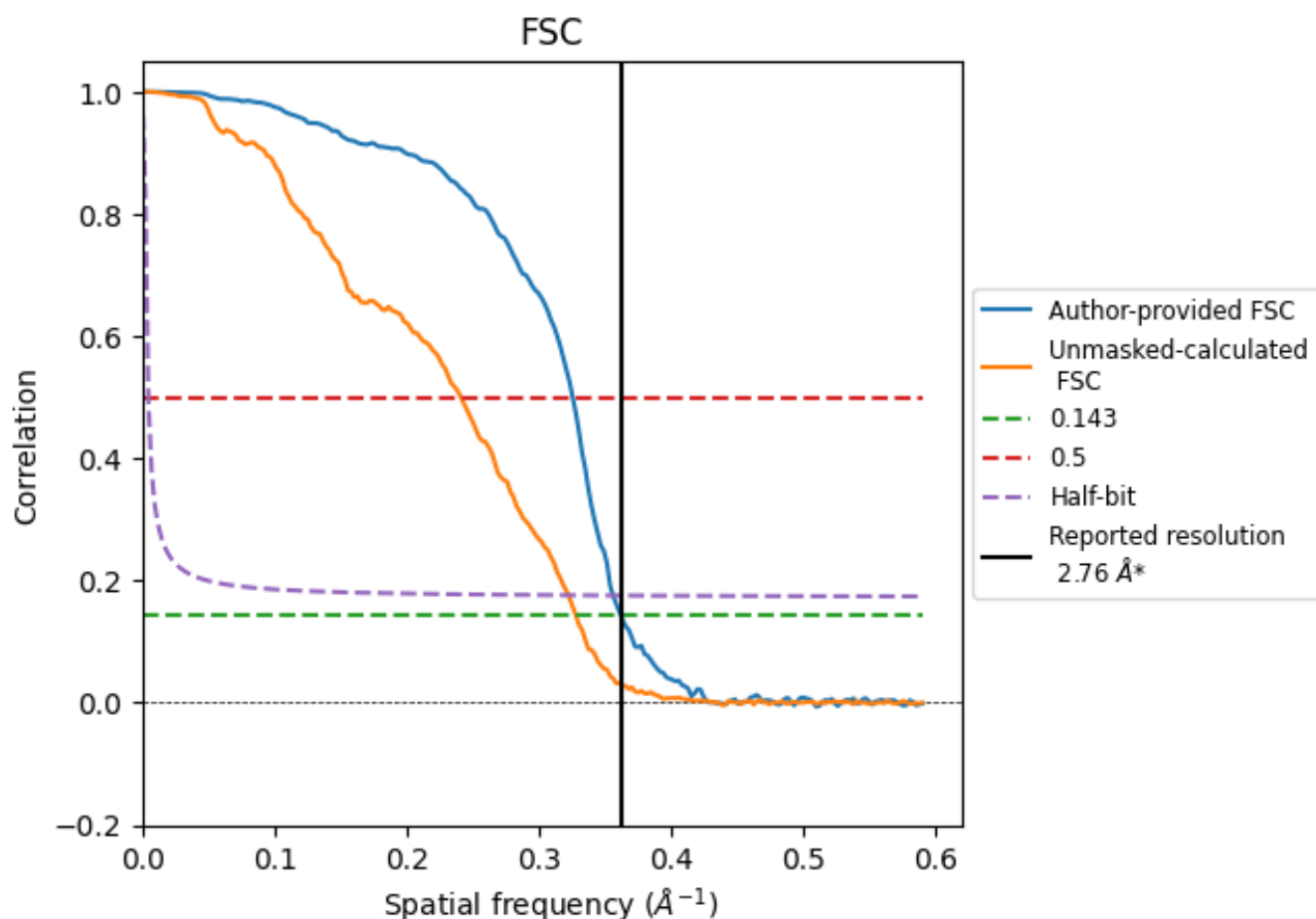


*Reported resolution corresponds to spatial frequency of 0.362 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.362 Å⁻¹

8.2 Resolution estimates [i](#)

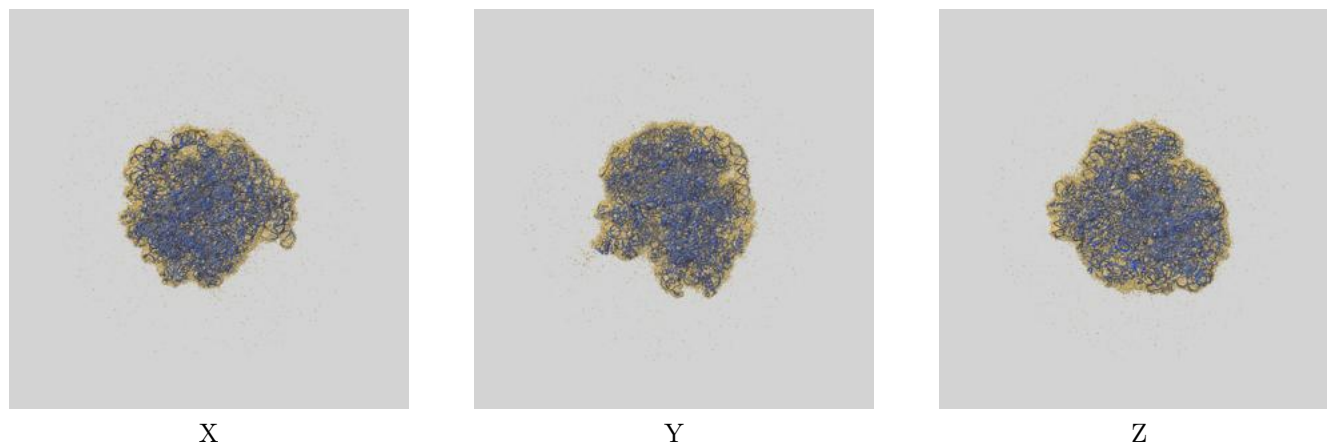
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.76	-	-
Author-provided FSC curve	2.76	3.07	2.81
Unmasked-calculated*	3.05	4.15	3.10

*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 3.05 differs from the reported value 2.76 by more than 10 %

9 Map-model fit [i](#)

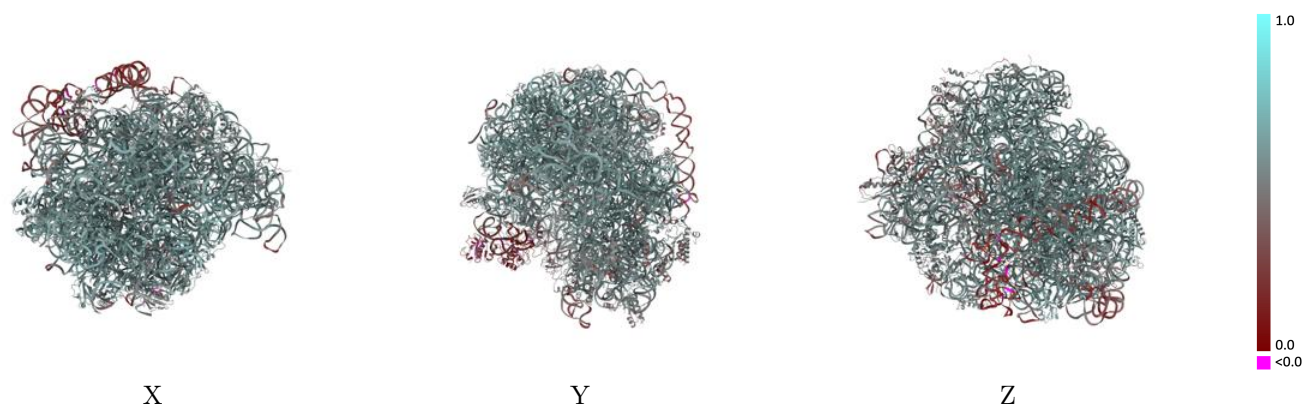
This section contains information regarding the fit between EMDB map EMD-29397 and PDB model 8FR8. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.003 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](#)

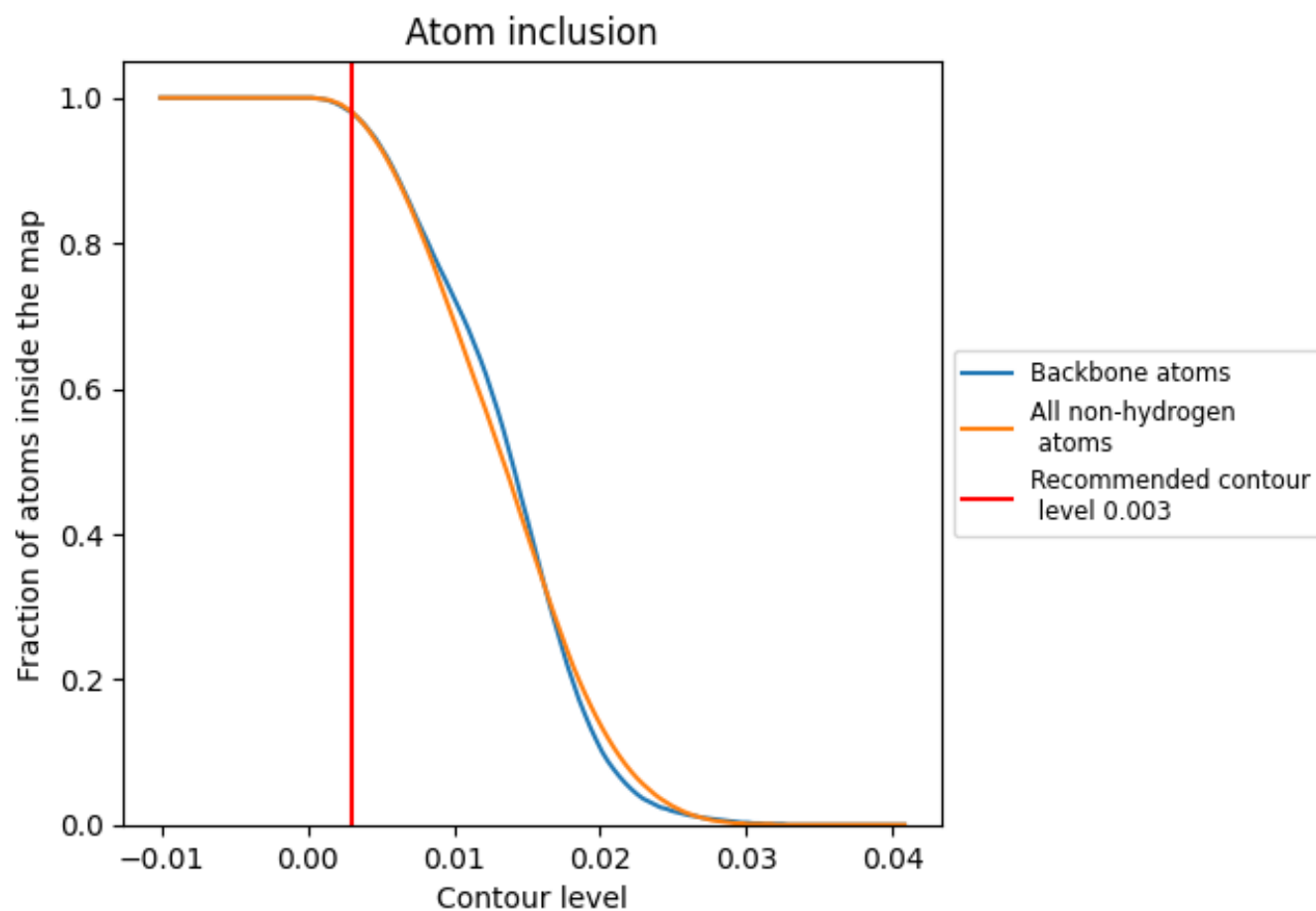


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 98% 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 (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9810	 0.5490
0	 1.0000	 0.6150
1	 0.9900	 0.5600
2	 0.9720	 0.5300
3	 0.9940	 0.6180
4	 1.0000	 0.6180
6	 0.9800	 0.5630
7	 0.9850	 0.5920
8	 0.9980	 0.5770
9	 0.9480	 0.4960
A	 0.9880	 0.5560
B	 0.9960	 0.5520
C	 0.9980	 0.5970
D	 0.9940	 0.5670
E	 0.9810	 0.4200
F	 1.0000	 0.6080
G	 0.9820	 0.5030
H	 0.8040	 0.4030
I	 0.4750	 0.2710
J	 0.9980	 0.6020
K	 0.9980	 0.6150
L	 0.9940	 0.5970
M	 0.9910	 0.5820
N	 0.9940	 0.5810
O	 0.9820	 0.5430
P	 0.9830	 0.5140
Q	 0.8880	 0.4680
R	 0.6230	 0.2390
S	 0.7840	 0.1930
T	 0.9950	 0.5960
U	 0.9980	 0.6000
V	 0.9970	 0.6010
W	 0.9910	 0.5960
X	 0.9880	 0.6000
Y	 0.9960	 0.5950



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Chain	Atom inclusion	Q-score
Z	 0.9910	 0.5620
a	 0.9980	 0.5680
b	 1.0000	 0.5870
c	 0.9700	 0.4690
d	 0.9800	 0.4800
e	 0.9830	 0.5000
f	 0.9760	 0.5450
g	 0.9800	 0.5400
h	 0.9950	 0.5260
i	 0.9960	 0.5800
j	 0.9800	 0.4960
k	 0.9910	 0.5440
l	 0.9640	 0.5090
m	 0.9950	 0.5600
n	 0.9940	 0.5660
o	 0.9940	 0.5030
p	 0.9910	 0.5700
q	 0.9790	 0.5400
r	 0.9930	 0.5620
t	 0.9890	 0.5430
u	 0.9440	 0.4680
v	 0.9850	 0.3500
x	 1.0000	 0.6210
y	 0.9220	 0.4750