



Full wwPDB EM Validation Report ⓘ

Jun 19, 2026 – 08:47 am BST

PDB ID : 5MDY / pdb_00005mdy
EMDB ID : EMD-3492
Title : Structure of ArfA and TtRF2 bound to the 70S ribosome (pre-accommodated state)
Authors : James, N.R.; Brown, A.; Gordiyenko, Y.; Ramakrishnan, V.
Deposited on : 2016-11-13
Resolution : 3.35 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:

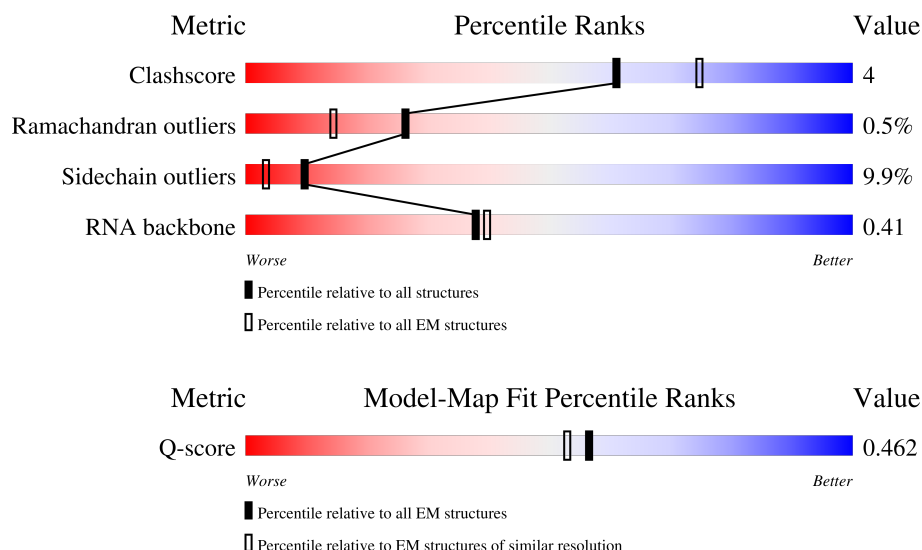
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.35 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	14390 (2.85 - 3.85)

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	1	2904	
2	2	1534	
3	3	120	

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Mol	Chain	Length	Quality of chain
4	4	18	
5	5	78	
6	6	61	
7	7	378	
8	B	273	
9	C	209	
10	D	201	
11	E	179	
12	F	177	
13	G	149	
14	H	165	
15	I	142	
16	J	142	
17	K	123	
18	L	144	
19	M	136	
20	N	127	
21	O	117	
22	P	115	
23	Q	118	
24	R	103	
25	S	110	
26	T	100	
27	U	104	
28	V	94	

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Mol	Chain	Length	Quality of chain
29	W	85	
30	X	78	
31	Y	63	
32	Z	59	
33	a	70	
34	b	57	
35	c	55	
36	d	46	
37	e	65	
38	f	38	
39	g	241	
40	h	233	
41	i	206	
42	j	167	
43	k	135	
44	l	179	
45	m	130	
46	n	130	
47	o	103	
48	p	129	
49	q	124	
50	r	118	
51	s	101	
52	t	89	
53	u	82	

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Mol	Chain	Length	Quality of chain
54	v	84	79%15%5%
55	w	75	71%12%5%12%
56	x	92	76%12%10%
57	y	87	87%11%
58	z	71	77%17%

2 Entry composition [i](#)

There are 62 unique types of molecules in this entry. The entry contains 149460 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	2903	Total	C	N	O	P	0	0
			62336	27816	11470	20147	2903		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	887	A	U	conflict	GB 802133627

- Molecule 2 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1534	Total	C	N	O	P	0	0
			32929	14693	6041	10661	1534		

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 4 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	5	Total	C	N	O	P	0	0
			109	49	22	33	5		

- Molecule 5 is a RNA chain called fMet-NH-tRNA(fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
5	5	76	Total	C	N	O	P	S	0	0
			1622	725	292	528	76	1		

- Molecule 6 is a protein called Alternative ribosome-rescue factor A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	32	Total	C	N	O	S	0	0
			259	163	53	42	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	0	HIS	-	expression tag	UNP P36675

- Molecule 7 is a protein called Peptide chain release factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	324	Total	C	N	O	S	0	0
			2597	1630	471	488	8		

- Molecule 8 is a protein called 50S ribosomal protein L2.

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

- Molecule 9 is a protein called 50S ribosomal protein L3.

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

- Molecule 10 is a protein called 50S ribosomal protein L4.

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

- Molecule 11 is a protein called 50S ribosomal protein L5.

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

- Molecule 12 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 13 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	146	Total	C	N	O	S	0	0
			1089	686	194	208	1		

- Molecule 14 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	130	Total	C	N	O	S	0	0
			980	620	174	182	4		

- Molecule 15 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	135	Total	C	N	O	S	0	0
			984	622	171	185	6		

- Molecule 16 is a protein called 50S ribosomal protein L13.

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

- Molecule 17 is a protein called 50S ribosomal protein L14.

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

- Molecule 18 is a protein called 50S ribosomal protein L15.

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

- Molecule 19 is a protein called 50S ribosomal protein L16.

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

- Molecule 20 is a protein called 50S ribosomal protein L17.

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

- Molecule 21 is a protein called 50S ribosomal protein L18.

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

- Molecule 22 is a protein called 50S ribosomal protein L19.

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

- Molecule 23 is a protein called 50S ribosomal protein L20.

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

- Molecule 24 is a protein called 50S ribosomal protein L21.

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

- Molecule 25 is a protein called 50S ribosomal protein L22.

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

- Molecule 26 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	94	Total	C	N	O	S	0	0
			746	470	140	134	2		

- Molecule 27 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	103	Total	C	N	O	S	0	0
			788	498	148	142			

- Molecule 28 is a protein called 50S ribosomal protein L25.

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

- Molecule 29 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 30 is a protein called 50S ribosomal protein L28.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Z	58	Total	C	N	O	S	0	0
			448	281	87	78	2		

- Molecule 33 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	63	Total	C	N	O	S	0	0
			495	304	95	90	6		

- Molecule 34 is a protein called 50S ribosomal protein L32.

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

- Molecule 35 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	c	52	Total	C	N	O	0	0
			426	275	78	73		

- Molecule 36 is a protein called 50S ribosomal protein L34.

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

- Molecule 37 is a protein called 50S ribosomal protein L35.

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

- Molecule 38 is a protein called 50S ribosomal protein L36.

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

- Molecule 39 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	225	Total	C	N	O	S	0	0
			1760	1113	316	323	8		

- Molecule 40 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	208	Total	C	N	O	S	0	0
			1636	1036	307	290	3		

- Molecule 41 is a protein called 30S ribosomal protein S4.

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

- Molecule 42 is a protein called 30S ribosomal protein S5.

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

- Molecule 43 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	k	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

- Molecule 44 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	l	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 45 is a protein called 30S ribosomal protein S8.

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

- Molecule 46 is a protein called 30S ribosomal protein S9.

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

- Molecule 47 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	o	99	Total	C	N	O	S	0	0
			790	495	151	143	1		

- Molecule 48 is a protein called 30S ribosomal protein S11.

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

- Molecule 49 is a protein called 30S ribosomal protein S12.

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

- Molecule 50 is a protein called 30S ribosomal protein S13.

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

- Molecule 51 is a protein called 30S ribosomal protein S14.

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

- Molecule 52 is a protein called 30S ribosomal protein S15.

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

- Molecule 53 is a protein called 30S ribosomal protein S16.

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

- Molecule 54 is a protein called 30S ribosomal protein S17.

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

- Molecule 55 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	w	66	Total	C	N	O	S	0	0
			544	344	102	97	1		

- Molecule 56 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	x	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 57 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	y	86	Total	C	N	O	S	0	0
			669	414	138	114	3		

- Molecule 58 is a protein called 30S ribosomal protein S21.

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

- Molecule 59 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

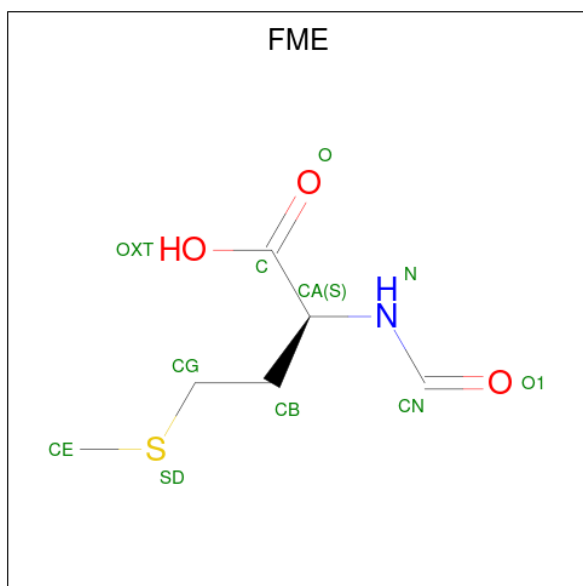
Mol	Chain	Residues	Atoms		AltConf
59	1	293	Total	Mg	0
			293	293	
59	2	143	Total	Mg	0
			143	143	
59	3	7	Total	Mg	0
			7	7	
59	5	4	Total	Mg	0
			4	4	
59	b	1	Total	Mg	0
			1	1	
59	f	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
59	i	1	Total	Mg	0
			1	1	

- Molecule 60 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
60	5	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
61	a	1	Total	Zn	0
			1	1	
61	f	1	Total	Zn	0
			1	1	

- Molecule 62 is water.

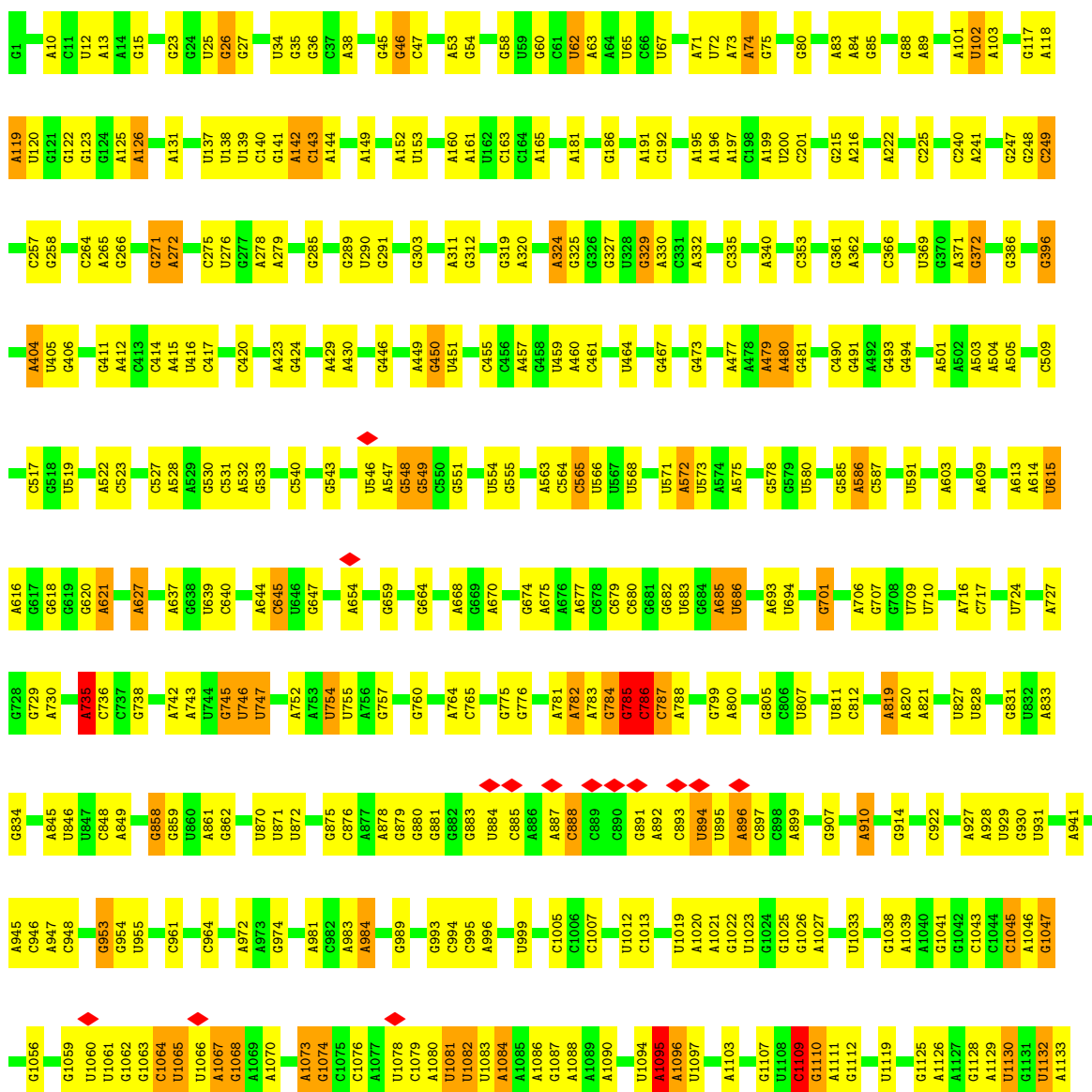
Mol	Chain	Residues	Atoms		AltConf
62	B	2	Total	O	0
			2	2	
62	O	1	Total	O	0
			1	1	

3 Residue-property plots

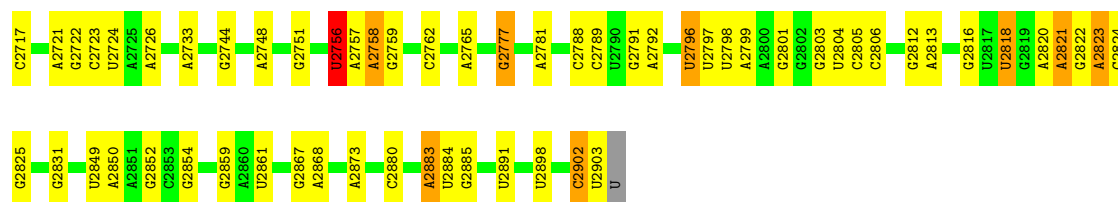
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 23S ribosomal RNA

Chain 1: 

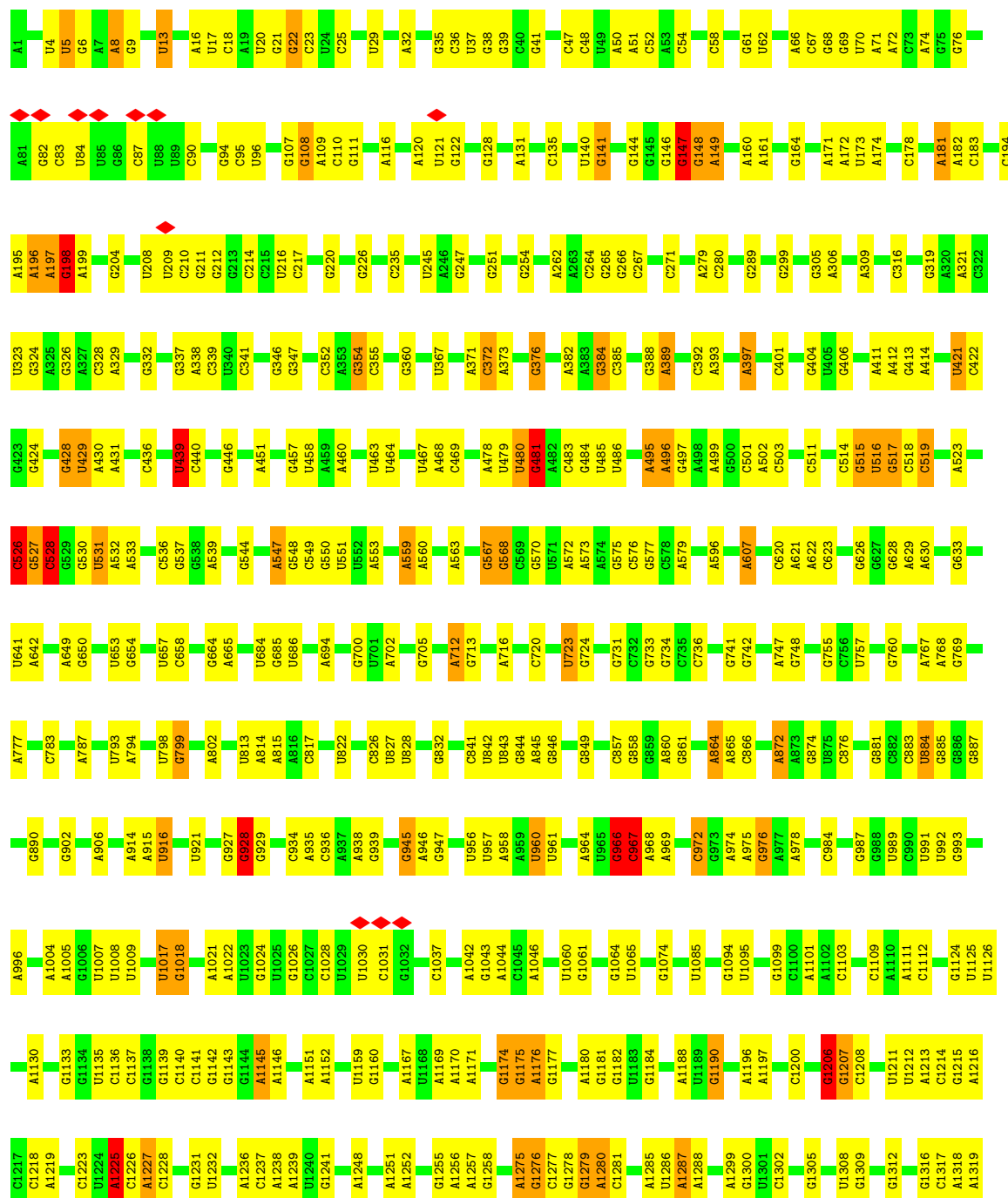


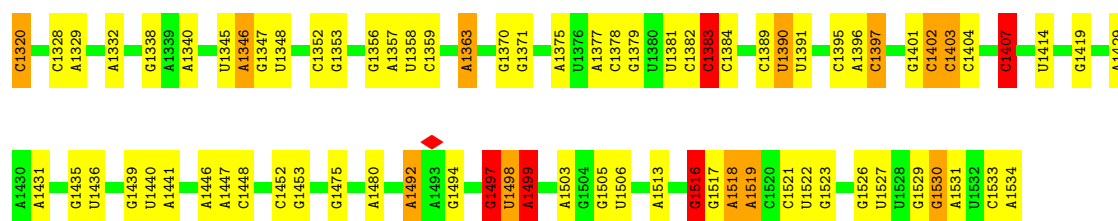
G2567	G2456	G2345	U2245	U2167	G2100	C2001	G1869	A1746	A1597	A1490	C1376	G1252	A1134
U2571	U2457	A2346	G2250	G2168	C2103	G2002	C1870	G1750	C1607	G1491	G1377	A1253	C1135
A2572	A2469	C2347	G2251	A2169	C2104	A2005	A1871	G1750	A1608	G1492	G1378	A1254	G1136
C2573	G2470	G2348	G2251	A2170	U2105	C2006	A1872	A1757	A1609	G1493	U1379	U1255	G1137
G2574	C2264	G2349	C2264	A2171	U2106	A2013	G1874	U1758	G1873	C1493	G1380	G1256	G1138
U2580	U2473	A2352	A2267	U2172	U2107	U2017	G1875	A1762	G1613	A1496	A1383	A1264	U1141
U2585	G2475	G2361	A2268	C2175	A2108	A2017	G1875	C1763	G1613	A1497	A1384	A1265	U1142
U2586	A2476	U2372	U2272	A2176	G2110	A2020	G1906	C1764	A1616	C1498	A1385	G1267	A1149
A2587	A2477	A2273	U2273	C2177	U2111	C2021	G1907	A1773	A1617	A1503	C1386	A1268	C1150
A2589	A2478	A2274	A2274	C2178	U2112	C2022	G1910	C1774	A1618	A1508	A1387	G1271	C1153
C2590	G2481	G2275	G2275	C2179	U2113	C2023	U1911	U1775	G1622	A1509	A1395	A1272	G1154
C2597	U2491	G2276	G2277	U2180	U2114	U2026	A1912	U1778	G1622	G1510	U1396	A1273	A1156
A2602	A2497	U2181	A2278	U2181	G2115	G2027	A1913	U1779	U1647	A1515	G1401	A1274	A1170
G2603	G2498	U2182	G2282	U2182	G2116	U2028	C1914	G1649	G1649	U1520	U1402	A1275	A1169
U2604	C2499	A2183	C2283	A2183	A2117	G2029	3TD1915	A1783	A1850	U1520	A1403	A1276	C1170
U2605	U2500	A2184	A2283	A2184	U2118	A2030	U1917	A1784	G1851	A1525	C1404	U1282	G1171
U2609	C2501	U2185	A2287	U2185	A2119	A2031	U1918	A1789	A1654	G1527	U1405	G1283	G1172
C2610	G2502	G2186	A2288	G2186	G2120	G2032	A1919	U1796	A1655	C1526	U1406	A1287	U1173
C2611	A2503	U2188	U2188	U2188	U2121	A2033	A1923	G1797	C1656	A1528	G1408	U1174	U1174
G2612	U2504	U2189	G2294	U2189	U2122	U2034	U1924	G1797	C1656	G1529	U1409	A1175	A1175
C2613	G2505	G2193	G2295	G2193	G2123	C2043	G1929	C1800	G1663	U1534	U1412	G1300	U1176
C2616	U2506	U2194	A2296	U2194	G2124	G2049	G1930	A1801	A1664	A1535	A1413	A1301	G1177
C2619	C2402	U2195	A2297	U2195	G2125	G2050	A1936	C1804	G1674	U1536	A1414	A1302	C1178
G2623	U2403	U2196	U2299	U2196	G2126	A2051	A1937	A1808	G1675	C1536	C1414	C1320	G1179
C2627	C2403	U2197	U2305	U2197	G2127	A2052	A1938	A1808	A1677	G1537	U1415	A1321	U1180
U2629	U2419	A2198	U2305	A2198	G2128	C2055	U1939	G1811	G1681	U1555	C1417	A1322	U1181
C2646	U2423	G2209	U2305	G2209	U2131	G2056	U1955	G1811	G1681	U1559	U1419	A1327	G1182
G2663	C2424	U2210	U2305	U2210	U2132	A2069	A1960	G1816	U1692	U1562	A1421	U1329	U1183
C2663	A2425	A2211	U2305	A2211	G2133	G2061	C1961	G1817	U1693	U1563	G1422	C1330	G1206
G2671	U2426	A2212	U2305	A2212	G2134	A2062	C1962	U1818	G1694	A1566	G1425	G1338	G1210
U2680	A2426	U2213	U2305	U2213	U2137	G2069	U1963	U1820	G1695	A1566	G1426	G1339	G1225
C2683	U2431	U2220	U2305	U2220	G2138	A2070	G1964	A1821	G1703	A1569	C1428	C1345	A1226
U2684	A2434	G2221	U2305	G2221	U2139	A2071	C1967	U1827	A1713	A1579	A1433	U1352	G1237
G2685	A2435	G2222	U2305	G2222	G2140	C2072	G1968	U1714	G1715	U1578	A1434	C1357	A1230
U2689	U2548	G2223	U2305	G2223	A2141	C2073	A1969	A1829	G1715	U1580	G1452	U1231	U1231
U2690	C2538	G2224	U2305	G2224	G2142	U2074	A1970	C1833	U1729	G1581	A1453	G1369	G1245
A2705	A2547	G2225	U2305	G2225	G2143	A2077	G1971	U1834	C1730	G1582	C1454	A1246	A1246
A2711	U2554	C2226	U2305	C2226	G2145	A2082	G1980	G1835	G1731	U1584	G1455	C1370	G1247
G2714	C2557	U2229	U2305	U2229	C2146	G2083	A1981	C1836	G1733	U1584	G1459	G1371	U1249
C2716	U2566	G2230	U2305	G2230	A2147	G2087	U1982	G1842	U1736	G1588	U1460	U1372	G1250
		U2231	U2305	U2231	G2154	G2093	U1991	A1847	G1737	U1589	A1469	G1369	G1251
		C2232	U2305	C2232	U2155	G2093	G1992	A1848	G1738	A1590	A1470	A1247	
		U2233	U2305	U2233	G2156	C2096	U1993	A1883	G1740	A1591	G1478	G1371	
		G2234	U2305	G2234	G2157	A2097	C1997	A1888	C1742	A1593	U1482	A1373	
		G2238	U2305	G2238	A2158	C2098	C1997	A1888	U1742	A1596			
		G2239	U2305	G2239	A2159	U2099	C2000	A1859					
		G2242	U2305	G2242	C2160								
		U2243	U2305	U2243	G2161								
		U2244	U2305	U2244	G2162								
			U2344		A2163								
					G2164								
					G2165								
					U2166								



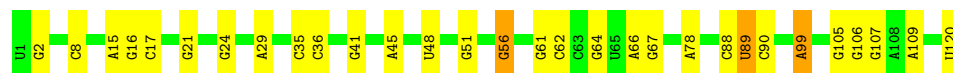
• Molecule 2: 16S ribosomal RNA

Chain 2: 64% 30% 5%





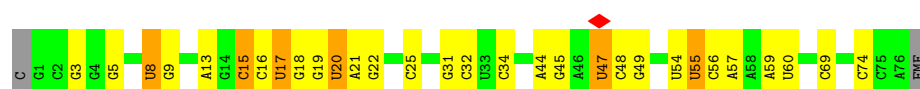
• Molecule 3: 5S ribosomal RNA



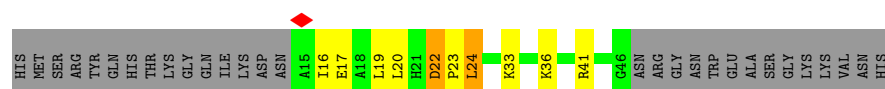
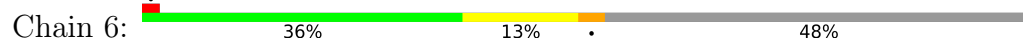
• Molecule 4: mRNA



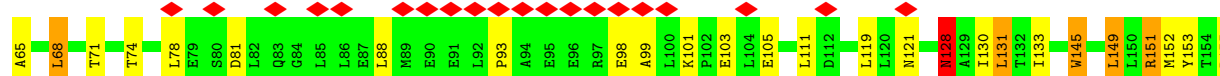
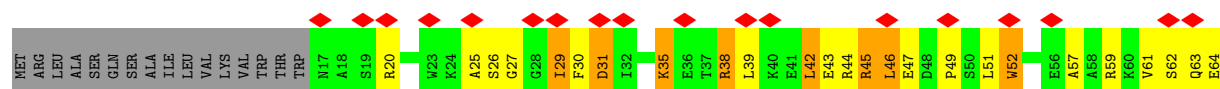
• Molecule 5: fMet-NH-tRNA(fMet)

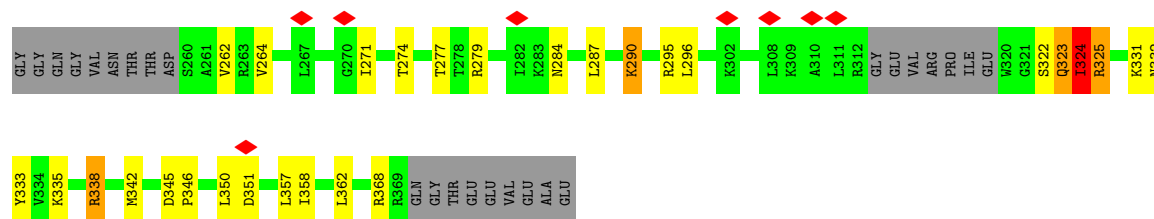


• Molecule 6: Alternative ribosome-rescue factor A



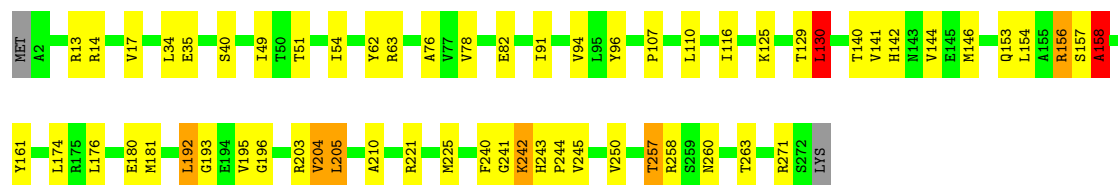
• Molecule 7: Peptide chain release factor 2





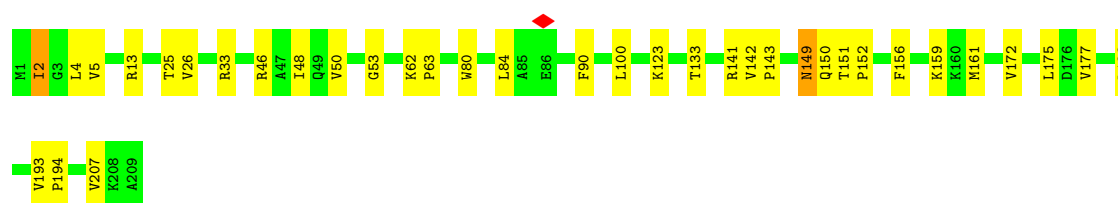
• Molecule 8: 50S ribosomal protein L2

Chain B: 77% 19% ..



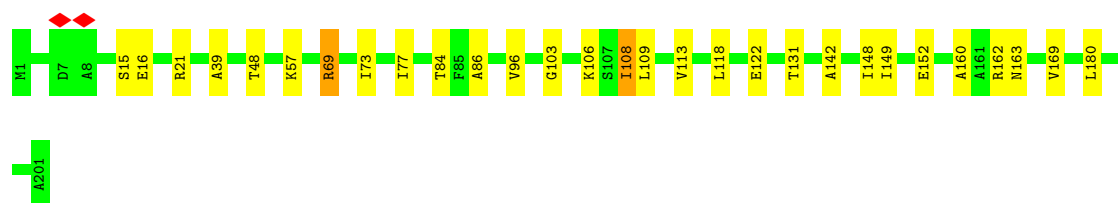
• Molecule 9: 50S ribosomal protein L3

Chain C: 83% 16% .



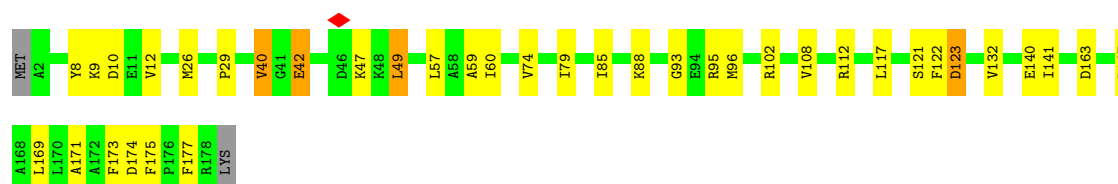
• Molecule 10: 50S ribosomal protein L4

Chain D: 85% 14% .



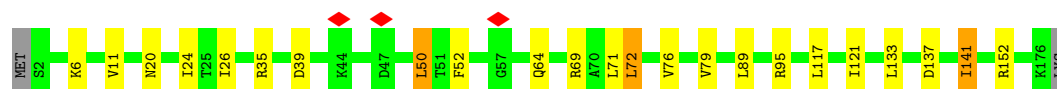
• Molecule 11: 50S ribosomal protein L5

Chain E: 78% 19% ..



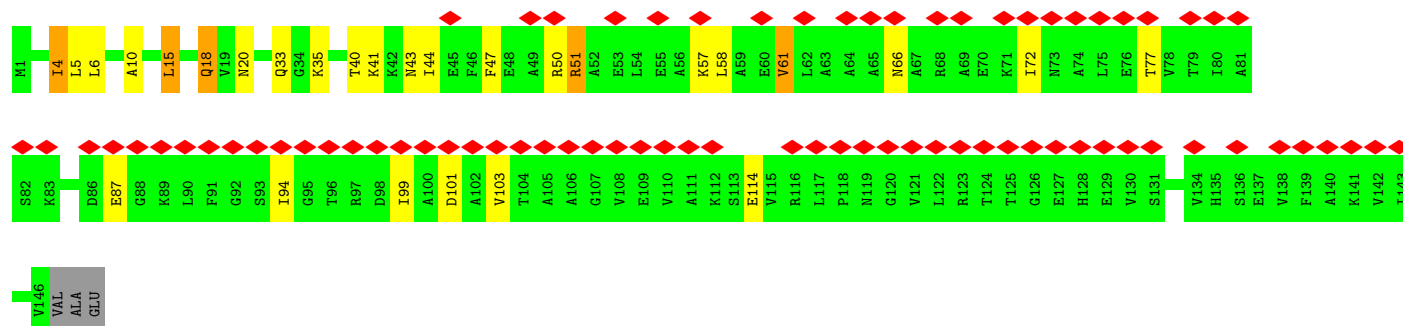
• Molecule 12: 50S ribosomal protein L6

Chain F: 



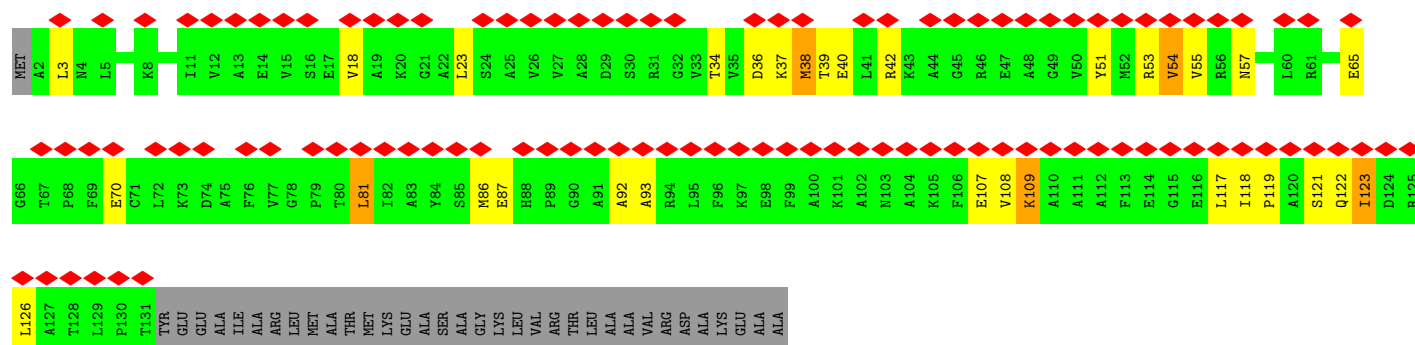
• Molecule 13: 50S ribosomal protein L9

Chain G: 



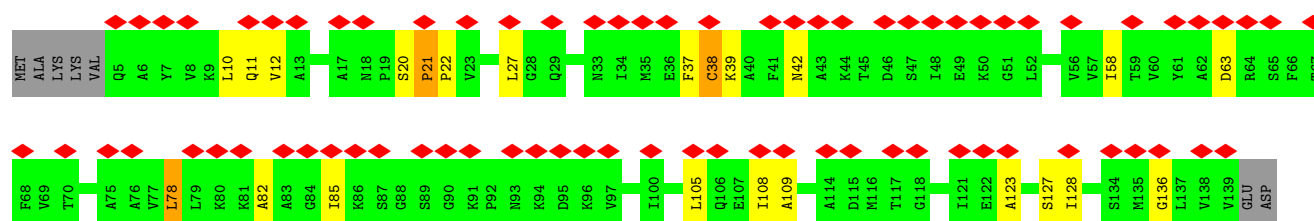
• Molecule 14: 50S ribosomal protein L10

Chain H: 



• Molecule 15: 50S ribosomal protein L11

Chain I: 



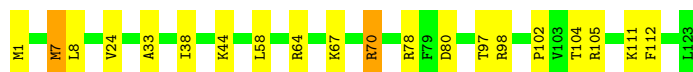
• Molecule 16: 50S ribosomal protein L13

Chain J: 



- Molecule 17: 50S ribosomal protein L14

Chain K: 84% 15% .



- Molecule 18: 50S ribosomal protein L15

Chain L: 81% 16% .



- Molecule 19: 50S ribosomal protein L16

Chain M: 82% 15% .



- Molecule 20: 50S ribosomal protein L17

Chain N: 70% 20% 6% .



- Molecule 21: 50S ribosomal protein L18

Chain O: 79% 19% ..



- Molecule 22: 50S ribosomal protein L19

Chain P: 81% 17% ..

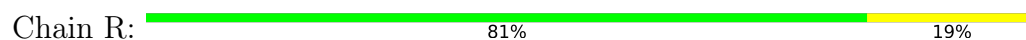


- Molecule 23: 50S ribosomal protein L20

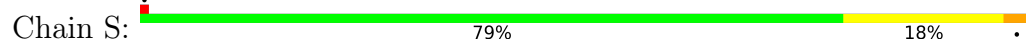
Chain Q: 77% 22% .



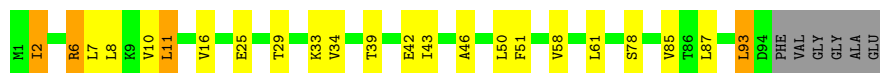
- Molecule 24: 50S ribosomal protein L21



- Molecule 25: 50S ribosomal protein L22



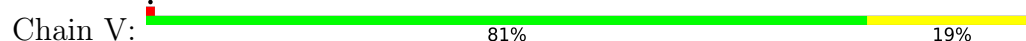
- Molecule 26: 50S ribosomal protein L23



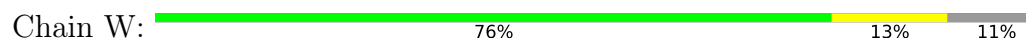
- Molecule 27: 50S ribosomal protein L24



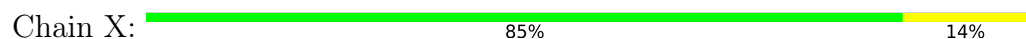
- Molecule 28: 50S ribosomal protein L25



- Molecule 29: 50S ribosomal protein L27



- Molecule 30: 50S ribosomal protein L28





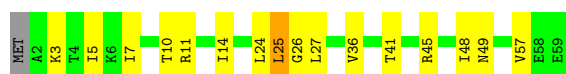
- Molecule 31: 50S ribosomal protein L29

Chain Y: 73% 24% ..



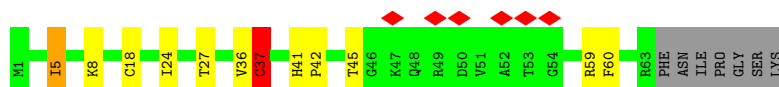
- Molecule 32: 50S ribosomal protein L30

Chain Z: 71% 25% ..



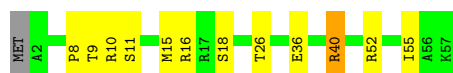
- Molecule 33: 50S ribosomal protein L31

Chain a: 9% 73% 14% .. 10%



- Molecule 34: 50S ribosomal protein L32

Chain b: 77% 19% ..



- Molecule 35: 50S ribosomal protein L33

Chain c: 73% 20% • 5%



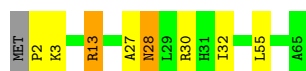
- Molecule 36: 50S ribosomal protein L34

Chain d: 76% 20% •



- Molecule 37: 50S ribosomal protein L35

Chain e: 86% 9% ..



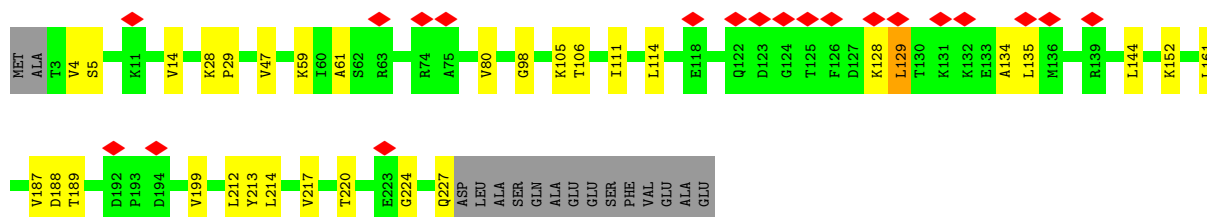
- Molecule 38: 50S ribosomal protein L36

Chain f: 79% 18%



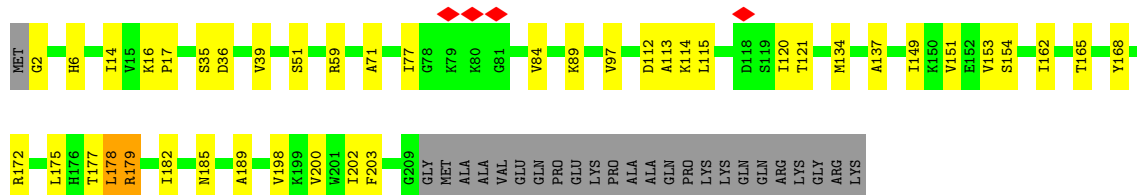
- Molecule 39: 30S ribosomal protein S2

Chain g: 8% 80% 13% 7%



- Molecule 40: 30S ribosomal protein S3

Chain h: 71% 17% 11%



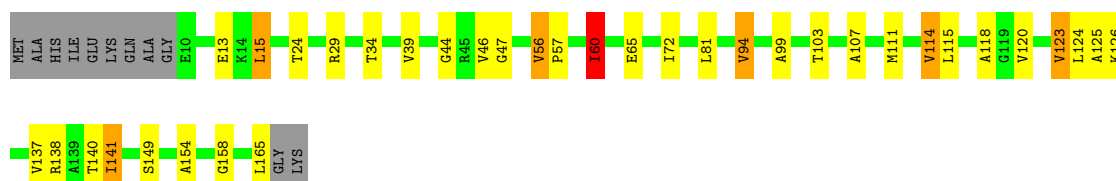
- Molecule 41: 30S ribosomal protein S4

Chain i: 86% 13%



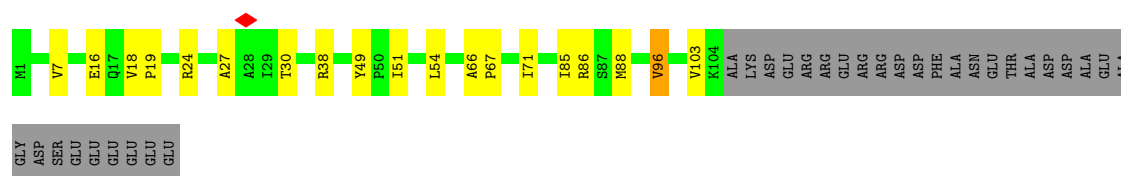
- Molecule 42: 30S ribosomal protein S5

Chain j: 72% 17% 7%



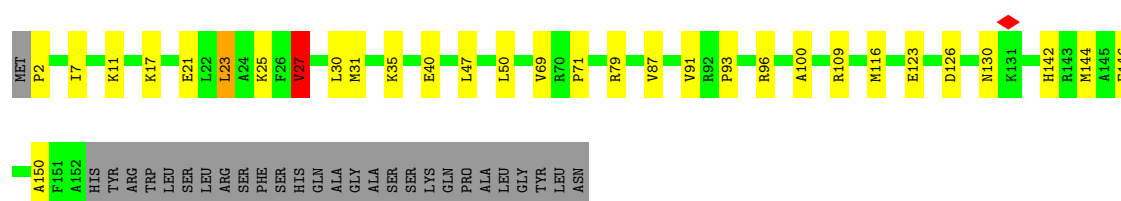
- Molecule 43: 30S ribosomal protein S6

Chain k:  63% 13% 23%



- Molecule 44: 30S ribosomal protein S7

Chain l:  67% 16% 16%



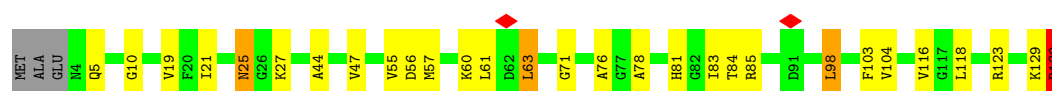
- Molecule 45: 30S ribosomal protein S8

Chain m:  89% 10%



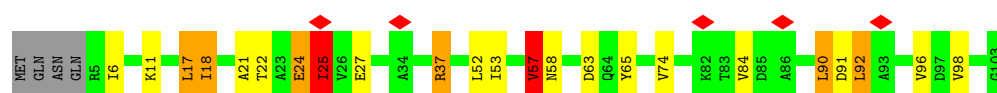
- Molecule 46: 30S ribosomal protein S9

Chain n:  75% 19%



- Molecule 47: 30S ribosomal protein S10

Chain o:  5% 74% 15% 6%



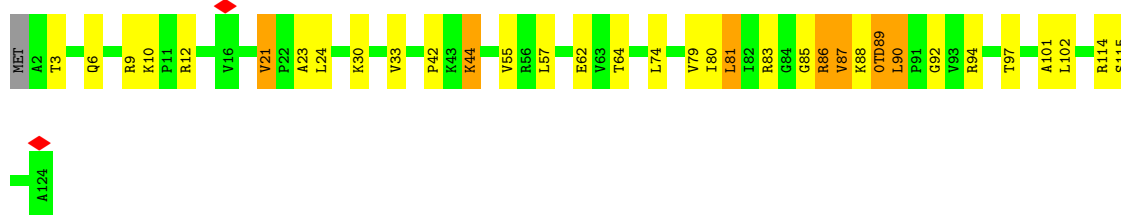
- Molecule 48: 30S ribosomal protein S11

Chain p:  77% 12% 9%



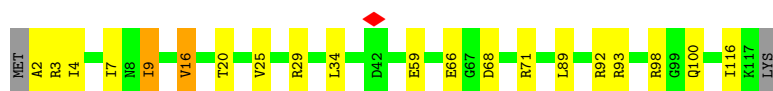
- Molecule 49: 30S ribosomal protein S12

Chain q:  72% 22% 6%



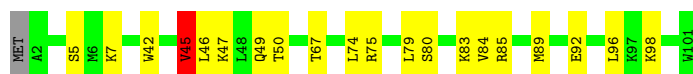
- Molecule 50: 30S ribosomal protein S13

Chain r:  81% 15%



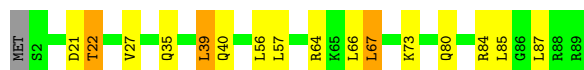
- Molecule 51: 30S ribosomal protein S14

Chain s:  79% 19%



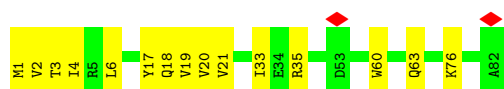
- Molecule 52: 30S ribosomal protein S15

Chain t:  81% 15%



- Molecule 53: 30S ribosomal protein S16

Chain u:  82% 18%



- Molecule 54: 30S ribosomal protein S17

Chain v:  79% 15% 5%



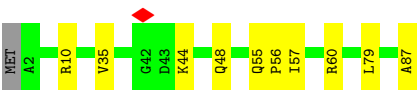
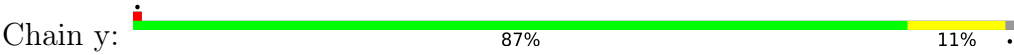
- Molecule 55: 30S ribosomal protein S18



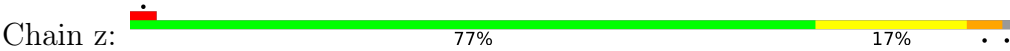
• Molecule 56: 30S ribosomal protein S19



• Molecule 57: 30S ribosomal protein S20



• Molecule 58: 30S ribosomal protein S21



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	54465	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 ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	134615	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.922	Depositor
Minimum map value	-0.590	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 4OC, 1MG, 3TD, 5MU, 2MA, 8AN, G7M, OMC, UR3, ZN, OMG, 4SU, 7MG, OMU, H2U, 6MZ, MA6, 0TD, PSU, 5MC, FME, 2MG

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	1	0.43	0/69285	0.84	144/108083 (0.1%)
2	2	0.41	0/36590	0.82	62/57074 (0.1%)
3	3	0.39	0/2872	0.73	1/4478 (0.0%)
4	4	0.43	0/122	0.83	0/188
5	5	0.42	0/1672	0.79	3/2603 (0.1%)
6	6	0.50	0/263	1.07	2/345 (0.6%)
7	7	0.73	0/2642	1.14	3/3563 (0.1%)
8	B	0.70	0/2121	1.00	6/2852 (0.2%)
9	C	0.70	0/1586	0.95	0/2134
10	D	0.66	0/1571	1.08	0/2113
11	E	0.62	0/1434	1.06	1/1926 (0.1%)
12	F	0.58	0/1333	0.96	0/1805
13	G	0.65	0/1100	1.02	1/1486 (0.1%)
14	H	0.72	0/993	1.06	1/1340 (0.1%)
15	I	0.68	0/998	1.07	1/1348 (0.1%)
16	J	0.68	0/1152	1.06	2/1551 (0.1%)
17	K	0.67	0/955	1.02	0/1279
18	L	0.66	0/1062	1.06	3/1413 (0.2%)
19	M	0.68	0/1093	0.99	0/1460
20	N	0.72	0/964	1.20	1/1289 (0.1%)
21	O	0.70	0/902	1.13	2/1209 (0.2%)
22	P	0.64	0/929	0.90	0/1242
23	Q	0.92	0/960	1.30	0/1278
24	R	0.55	0/829	0.85	0/1107
25	S	0.76	0/864	1.10	0/1156
26	T	0.65	0/752	0.96	0/1005
27	U	0.51	0/796	0.82	0/1062
28	V	0.58	0/766	0.92	0/1025
29	W	0.68	0/589	0.90	1/779 (0.1%)
30	X	0.70	0/635	1.05	0/848
31	Y	0.71	0/502	1.25	0/667

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Z	0.60	0/452	1.04	0/605
33	a	0.57	0/503	1.04	3/671 (0.4%)
34	b	0.67	0/450	0.97	0/599
35	c	0.57	0/433	0.87	0/576
36	d	0.79	0/380	1.18	0/498
37	e	0.71	0/513	1.16	1/676 (0.1%)
38	f	0.61	0/303	0.98	0/397
39	g	0.62	0/1791	1.08	1/2413 (0.0%)
40	h	0.61	0/1663	1.02	1/2241 (0.0%)
41	i	0.65	0/1665	1.11	5/2227 (0.2%)
42	j	0.72	0/1165	1.14	2/1568 (0.1%)
43	k	0.62	0/867	1.03	0/1171
44	l	0.69	0/1195	1.22	2/1602 (0.1%)
45	m	0.63	0/989	0.97	0/1326
46	n	0.60	0/1034	1.06	1/1375 (0.1%)
47	o	0.56	0/800	1.05	2/1082 (0.2%)
48	p	0.59	0/893	0.97	0/1205
49	q	0.60	0/960	0.97	5/1286 (0.4%)
50	r	0.67	0/909	1.16	0/1215
51	s	0.66	0/817	1.12	1/1088 (0.1%)
52	t	0.70	0/722	1.20	1/964 (0.1%)
53	u	0.66	0/659	1.02	0/884
54	v	0.53	0/657	0.82	0/881
55	w	0.65	0/553	1.12	1/743 (0.1%)
56	x	0.53	0/680	0.92	0/915
57	y	0.80	0/675	1.36	0/895
58	z	0.70	0/597	1.18	1/792 (0.1%)
All	All	0.51	0/160657	0.90	261/239603 (0.1%)

There are no bond length outliers.

All (261) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1276	G	C1'-C2'-O2'	-12.75	89.28	108.40
1	1	1914	C	C4'-C3'-O3'	12.56	131.84	113.00
1	1	1913	A	C4'-C3'-O3'	11.94	127.30	109.40
1	1	786	C	N1-C1'-C2'	-10.09	96.86	112.00
1	1	2017	U	C2'-C3'-O3'	-9.81	98.99	113.70
1	1	2071	A	C4'-C3'-O3'	-9.76	98.36	113.00
1	1	2296	U	C4'-C3'-O3'	9.62	123.84	109.40
2	2	928	G	C4'-C3'-O3'	9.60	127.41	113.00
2	2	1277	C	N1-C1'-C2'	-9.57	97.64	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	927	G	C1'-C2'-O2'	-9.49	94.16	108.40
2	2	928	G	N9-C1'-C2'	-9.18	98.23	112.00
1	1	2272	U	C2'-C3'-O3'	-8.85	100.42	113.70
1	1	1923	U	C4'-C3'-O3'	8.83	126.24	113.00
1	1	1405	U	C1'-C2'-O2'	-8.78	95.23	108.40
2	2	927	G	C4'-C3'-O3'	8.72	126.08	113.00
18	L	36	LYS	N-CA-C	8.67	123.33	111.54
2	2	198	G	C4'-C3'-O3'	8.44	125.66	113.00
2	2	1206	G	C4'-C3'-O3'	8.38	125.57	113.00
1	1	404	A	C2'-C3'-O3'	8.33	122.00	109.50
51	s	45	VAL	N-CA-CB	8.29	120.24	110.55
1	1	1404	C	C1'-C2'-O2'	-8.26	96.02	108.40
2	2	428	G	C4'-C3'-O3'	8.25	121.77	109.40
2	2	1401	G	C4'-C3'-O3'	8.22	125.33	113.00
2	2	198	G	N9-C1'-C2'	-7.97	100.05	112.00
2	2	1401	G	N9-C1'-C2'	-7.95	100.08	112.00
1	1	2193	G	C2'-C3'-O3'	7.90	125.56	113.70
1	1	2186	G	C4'-C3'-O3'	7.88	124.81	113.00
1	1	2602	A	C4'-C3'-O3'	7.87	121.20	109.40
2	2	1391	U	N1-C1'-C2'	-7.85	100.23	112.00
1	1	2425	A	C2'-C3'-O3'	7.81	121.21	109.50
2	2	528	C	N1-C1'-C2'	-7.78	100.33	112.00
47	o	57	VAL	N-CA-C	7.76	125.47	109.34
1	1	675	A	C4'-C3'-O3'	-7.57	101.65	113.00
2	2	927	G	N9-C1'-C2'	-7.55	100.67	112.00
2	2	1276	G	C4'-C3'-O3'	7.52	124.28	113.00
42	j	60	ILE	N-CA-CB	7.51	119.34	110.55
2	2	1384	C	N1-C1'-C2'	-7.42	100.87	112.00
2	2	1391	U	C4'-C3'-O3'	7.41	124.11	113.00
11	E	108	VAL	O-C-N	7.41	125.33	120.07
1	1	1406	U	N1-C1'-C2'	-7.39	100.91	112.00
2	2	1499	A	N9-C1'-C2'	-7.39	100.92	112.00
1	1	994	C	C4'-C3'-O3'	-7.30	102.05	113.00
1	1	2162	G	C4'-C3'-O3'	7.26	120.30	109.40
1	1	2506	U	C4'-C3'-O3'	7.15	120.12	109.40
1	1	786	C	C4'-C3'-O3'	7.15	123.72	113.00
42	j	56	VAL	O-C-N	7.14	124.99	120.42
44	l	27	VAL	N-CA-CB	7.14	118.91	110.55
1	1	896	A	C4'-C3'-O3'	7.13	120.10	109.40
18	L	35	HIS	N-CA-C	7.13	120.55	109.07
7	7	345	ASP	CA-C-N	7.10	127.42	119.32
7	7	345	ASP	C-N-CA	7.10	127.42	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1154	G	C2'-C3'-O3'	-7.06	103.11	113.70
5	5	47	U	C2'-C3'-O3'	7.05	120.08	109.50
1	1	1252	G	C3'-C2'-O2'	-7.03	104.06	114.60
2	2	1206	G	N9-C1'-C2'	-7.02	101.47	112.00
2	2	864	A	N9-C1'-C2'	7.00	122.51	112.00
39	g	47	VAL	O-C-N	6.94	124.86	120.42
2	2	515	G	C4'-C3'-O3'	6.93	123.39	113.00
1	1	1404	C	C4'-C3'-O3'	6.92	123.38	113.00
1	1	2756	U	C4'-C3'-O3'	6.80	119.60	109.40
6	6	22	ASP	CA-C-N	6.79	126.59	119.05
6	6	22	ASP	C-N-CA	6.79	126.59	119.05
2	2	1208	C	N1-C1'-C2'	-6.72	101.92	112.00
1	1	249	C	C2'-C3'-O3'	-6.72	99.42	109.50
2	2	354	G	C4'-C3'-O3'	-6.66	103.01	113.00
2	2	1383	C	N1-C1'-C2'	-6.62	102.07	112.00
15	I	21	PRO	N-CA-C	6.61	118.77	110.70
2	2	148	G	N9-C1'-C2'	-6.60	102.10	112.00
1	1	858	G	C2'-C3'-O3'	6.58	119.37	109.50
13	G	61	VAL	N-CA-CB	6.57	118.23	110.55
1	1	894	U	C2'-C3'-O3'	6.55	119.33	109.50
49	q	87	VAL	N-CA-C	-6.52	98.25	108.23
1	1	1331	G	C4'-C3'-O3'	-6.50	103.25	113.00
1	1	1095	A	C4'-C3'-O3'	6.48	119.12	109.40
5	5	17	U	C2'-C3'-O3'	6.43	119.15	109.50
1	1	2777	G	C2'-C3'-O3'	-6.43	104.06	113.70
1	1	1692	U	C4'-C3'-O3'	-6.41	103.38	113.00
1	1	1910	G	C4'-C3'-O3'	6.40	122.60	113.00
1	1	2796	U	C4'-C3'-O3'	6.40	119.00	109.40
1	1	126	A	C4'-C3'-O3'	-6.38	103.42	113.00
1	1	754	U	N1-C1'-C2'	6.37	121.55	112.00
1	1	1379	U	C2'-C3'-O3'	6.35	123.22	113.70
2	2	1390	U	C4'-C3'-O3'	6.35	122.52	113.00
2	2	1431	A	C4'-C3'-O3'	-6.27	103.60	113.00
1	1	1834	U	C4'-C3'-O3'	-6.25	103.63	113.00
1	1	2034	U	C4'-C3'-O3'	-6.25	103.63	113.00
1	1	2434	A	C2'-C3'-O3'	-6.22	104.37	113.70
37	e	13	ARG	N-CA-C	6.22	120.60	112.89
1	1	2315	G	N9-C1'-C2'	-6.18	102.73	112.00
1	1	329	G	C4'-C3'-O3'	-6.16	100.16	109.40
1	1	479	A	C4'-C3'-O3'	6.15	118.63	109.40
1	1	247	G	C4'-C3'-O3'	-6.13	103.80	113.00
1	1	2823	A	C4'-C3'-O3'	-6.13	103.80	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	o	25	ILE	N-CA-CB	6.11	117.70	110.55
1	1	2349	G	C4'-C3'-O3'	-6.10	103.85	113.00
1	1	677	A	C1'-C2'-O2'	6.08	117.53	108.40
1	1	953	G	C1'-C2'-O2'	6.07	117.51	108.40
1	1	1328	A	C4'-C3'-O3'	-6.07	103.90	113.00
41	i	6	GLY	CA-C-N	6.04	126.39	119.93
41	i	6	GLY	C-N-CA	6.04	126.39	119.93
1	1	2186	G	C2'-C3'-O3'	-6.02	104.67	113.70
1	1	2072	C	C4'-C3'-O3'	-6.01	103.98	113.00
1	1	1969	A	C4'-C3'-O3'	-6.01	103.98	113.00
1	1	1095	A	C1'-C2'-O2'	-6.00	102.80	111.80
1	1	195	A	C4'-C3'-O3'	-6.00	104.00	113.00
2	2	481	G	C2'-C3'-O3'	-5.99	100.51	109.50
7	7	324	ILE	N-CA-C	-5.99	105.29	110.74
2	2	526	C	N1-C1'-C2'	-5.99	103.02	112.00
1	1	1254	A	C4'-C3'-O3'	-5.97	104.04	113.00
2	2	480	U	C4'-C3'-O3'	5.88	121.82	113.00
2	2	883	C	C4'-C3'-O3'	-5.85	104.23	113.00
2	2	1208	C	C4'-C3'-O3'	5.84	121.77	113.00
1	1	38	A	C4'-C3'-O3'	-5.82	104.27	113.00
18	L	22	GLY	N-CA-C	5.81	118.80	112.29
2	2	1276	G	N9-C1'-C2'	-5.81	103.29	112.00
1	1	1914	C	C2'-C3'-O3'	-5.81	104.99	113.70
2	2	1346	A	C4'-C3'-O3'	-5.77	100.75	109.40
33	a	37	CYS	CA-CB-SG	-5.77	101.14	114.40
1	1	13	A	C2'-C3'-O3'	5.76	118.14	109.50
1	1	2026	U	C1'-C2'-O2'	5.75	117.03	108.40
1	1	2616	C	C3'-C2'-O2'	5.74	119.31	110.70
1	1	785	G	C1'-C2'-O2'	-5.74	99.80	108.40
1	1	787	C	C4'-C3'-O3'	-5.73	104.41	113.00
2	2	1391	U	C2'-C3'-O3'	-5.73	105.11	113.70
1	1	1045	C	C2'-C3'-O3'	-5.72	105.12	113.70
1	1	2436	G	N9-C1'-C2'	-5.71	103.43	112.00
1	1	2394	C	C4'-C3'-O3'	-5.70	104.45	113.00
21	O	74	VAL	CA-C-N	5.68	126.25	119.94
21	O	74	VAL	C-N-CA	5.68	126.25	119.94
2	2	550	G	C3'-C2'-O2'	5.67	119.21	110.70
1	1	1970	A	C2'-C3'-O3'	5.67	118.00	109.50
14	H	81	LEU	N-CA-C	5.65	119.48	112.24
1	1	2792	A	C4'-C3'-O3'	-5.64	104.55	113.00
8	B	243	HIS	CA-C-N	5.63	125.65	119.90
8	B	243	HIS	C-N-CA	5.63	125.65	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2315	G	C4'-C3'-O3'	5.63	121.45	113.00
2	2	1383	C	C4'-C3'-O3'	5.63	121.45	113.00
1	1	1405	U	C3'-C2'-O2'	5.62	119.13	110.70
1	1	2587	A	C2'-C3'-O3'	-5.61	105.29	113.70
55	w	16	GLU	N-CA-C	-5.61	105.17	111.28
1	1	2225	A	C4'-C3'-O3'	5.60	117.80	109.40
1	1	2425	A	C4'-C3'-O3'	5.59	117.78	109.40
2	2	147	G	C1'-C2'-O2'	-5.57	100.04	108.40
46	n	130	ARG	NE-CZ-NH2	5.57	124.21	119.20
1	1	2597	G	C4'-C3'-O3'	-5.57	104.65	113.00
1	1	2818	U	C3'-C2'-O2'	5.55	119.02	110.70
1	1	2231	U	C1'-C2'-O2'	5.54	116.71	108.40
1	1	2343	U	C4'-C3'-O3'	-5.54	104.69	113.00
1	1	25	U	C4'-C3'-O3'	-5.53	104.70	113.00
1	1	2680	U	C4'-C3'-O3'	-5.52	104.72	113.00
1	1	2020	A	C4'-C3'-O3'	-5.52	104.73	113.00
1	1	1875	G	C4'-C3'-O3'	-5.51	104.74	113.00
1	1	473	G	C4'-C3'-O3'	-5.50	104.75	113.00
2	2	720	C	C4'-C3'-O3'	-5.48	104.78	113.00
40	h	39	VAL	N-CA-CB	5.48	116.97	110.55
1	1	701	G	C4'-C3'-O3'	-5.47	104.79	113.00
1	1	2723	C	C4'-C3'-O3'	-5.47	104.80	113.00
1	1	1676	A	C4'-C3'-O3'	-5.45	104.83	113.00
1	1	1141	U	N1-C1'-C2'	5.45	122.17	114.00
1	1	2717	C	C1'-C2'-O2'	5.45	116.57	108.40
8	B	130	LEU	CA-C-N	5.45	125.44	119.89
8	B	130	LEU	C-N-CA	5.45	125.44	119.89
1	1	2308	G	C2'-C3'-O3'	-5.44	105.54	113.70
1	1	2724	U	C4'-C3'-O3'	-5.44	104.84	113.00
1	1	26	G	C4'-C3'-O3'	-5.42	104.86	113.00
1	1	528	A	C4'-C3'-O3'	-5.42	104.87	113.00
1	1	2005	A	C2'-C3'-O3'	-5.42	105.57	113.70
20	N	38	LEU	O-C-N	5.42	124.66	120.38
1	1	578	G	C4'-C3'-O3'	-5.42	104.88	113.00
49	q	92	GLY	N-CA-C	5.42	123.51	113.76
1	1	2411	A	C4'-C3'-O3'	-5.40	104.90	113.00
49	q	44	LYS	N-CA-C	5.39	115.80	109.60
49	q	90	LEU	CA-C-N	-5.39	114.37	119.76
49	q	90	LEU	C-N-CA	-5.39	114.37	119.76
1	1	1971	U	C4'-C3'-O3'	-5.39	104.92	113.00
2	2	1145	A	C4'-C3'-O3'	-5.39	104.92	113.00
1	1	2377	A	C3'-C2'-O2'	5.38	118.76	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	158	ALA	N-CA-C	5.37	122.23	110.80
1	1	1025	G	C4'-C3'-O3'	5.35	117.43	109.40
1	1	2538	C	C3'-C2'-O2'	5.35	118.73	110.70
3	3	41	G	C4'-C3'-O3'	-5.35	104.97	113.00
2	2	1190	G	C4'-C3'-O3'	-5.35	101.38	109.40
1	1	2711	A	C4'-C3'-O3'	-5.34	104.98	113.00
1	1	2500	U	C2'-C3'-O3'	-5.34	105.69	113.70
1	1	1132	U	C2'-C3'-O3'	5.34	117.51	109.50
1	1	2551	C	C4'-C3'-O3'	-5.34	104.99	113.00
1	1	2721	A	C1'-C2'-O2'	5.33	116.40	108.40
1	1	449	A	C4'-C3'-O3'	-5.33	105.00	113.00
1	1	781	A	C4'-C3'-O3'	-5.32	105.03	113.00
1	1	727	A	C4'-C3'-O3'	-5.30	105.04	113.00
1	1	2242	G	C1'-C2'-O2'	5.30	116.36	108.40
1	1	735	A	C3'-C2'-O2'	5.30	118.65	110.70
1	1	2029	G	C1'-C2'-O2'	5.30	116.34	108.40
44	1	31	MET	N-CA-C	5.30	117.12	110.24
2	2	1395	C	C4'-C3'-O3'	-5.28	105.08	113.00
1	1	1174	U	C2'-C3'-O3'	-5.27	105.79	113.70
1	1	1757	A	C4'-C3'-O3'	-5.27	105.09	113.00
1	1	1255	U	C4'-C3'-O3'	-5.26	105.11	113.00
1	1	2436	G	C4'-C3'-O3'	5.26	120.89	113.00
2	2	13	U	C2'-C3'-O3'	5.25	117.38	109.50
33	a	5	ILE	N-CA-C	5.25	116.61	110.62
2	2	1180	A	C4'-C3'-O3'	-5.25	105.13	113.00
2	2	1319	A	C2'-C3'-O3'	5.25	117.37	109.50
1	1	1376	C	C2'-C3'-O3'	-5.24	105.83	113.70
33	a	37	CYS	N-CA-C	-5.24	101.74	109.18
58	z	42	THR	CB-CA-C	-5.24	102.65	110.88
1	1	2419	U	C3'-C2'-O2'	5.23	118.54	110.70
1	1	2210	U	C4'-C3'-O3'	5.22	117.23	109.40
1	1	2619	C	C4'-C3'-O3'	-5.21	105.18	113.00
2	2	1497	G	C4'-C3'-O3'	5.21	120.82	113.00
1	1	1373	A	C4'-C3'-O3'	-5.21	105.19	113.00
16	J	112	GLY	CA-C-N	5.21	126.35	119.84
16	J	112	GLY	C-N-CA	5.21	126.35	119.84
1	1	1235	G	C4'-C3'-O3'	-5.21	105.19	113.00
1	1	2531	A	C4'-C3'-O3'	-5.20	105.19	113.00
1	1	564	C	C1'-C2'-O2'	5.18	116.17	108.40
2	2	25	C	C3'-C2'-O2'	5.18	118.47	110.70
1	1	240	C	C4'-C3'-O3'	-5.17	105.25	113.00
41	i	69	GLU	CA-C-O	-5.16	115.39	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	65	U	C1'-C2'-O2'	5.15	116.13	108.40
1	1	73	A	C2'-C3'-O3'	-5.14	106.00	113.70
2	2	147	G	C4'-C3'-O3'	5.13	120.70	113.00
2	2	1384	C	C4'-C3'-O3'	5.12	120.68	113.00
2	2	235	C	C3'-C2'-O2'	5.12	118.38	110.70
2	2	1237	C	C4'-C3'-O3'	-5.12	105.32	113.00
2	2	1497	G	N9-C1'-C2'	-5.12	104.32	112.00
2	2	1527	U	C4'-C3'-O3'	-5.12	105.33	113.00
1	1	2229	U	C1'-C2'-O2'	5.11	116.06	108.40
5	5	15	C	C2'-C3'-O3'	5.11	117.16	109.50
1	1	527	C	C2'-C3'-O3'	-5.10	101.85	109.50
2	2	1225	A	C4'-C3'-O3'	5.10	117.05	109.40
1	1	565	C	C4'-C3'-O3'	-5.10	105.35	113.00
1	1	1078	U	C2'-C3'-O3'	-5.10	106.05	113.70
1	1	760	G	C3'-C2'-O2'	5.10	118.34	110.70
1	1	2831	G	C4'-C3'-O3'	-5.09	105.36	113.00
1	1	2275	C	C2'-C3'-O3'	5.09	117.13	109.50
1	1	2590	A	C3'-C2'-O2'	5.08	118.32	110.70
1	1	1555	G	C4'-C3'-O3'	-5.07	105.39	113.00
2	2	712	A	C4'-C3'-O3'	-5.07	105.39	113.00
2	2	783	C	C4'-C3'-O3'	-5.07	105.39	113.00
2	2	1533	C	C4'-C3'-O3'	5.07	117.00	109.40
1	1	2428	G	C2'-C3'-O3'	-5.07	106.10	113.70
8	B	49	ILE	CB-CA-C	-5.06	105.16	111.08
1	1	1109	C	C2'-C3'-O3'	5.05	117.08	109.50
1	1	1762	A	C4'-C3'-O3'	-5.05	105.42	113.00
1	1	1527	G	C2'-C3'-O3'	-5.04	106.14	113.70
1	1	1775	U	C1'-C2'-O2'	5.04	115.96	108.40
29	W	44	LYS	N-CA-C	-5.04	105.86	111.36
1	1	1779	U	C4'-C3'-O3'	-5.04	105.45	113.00
1	1	972	A	C4'-C3'-O3'	-5.03	105.45	113.00
2	2	884	U	N1-C1'-C2'	5.03	121.55	114.00
1	1	423	A	C2'-C3'-O3'	-5.03	106.16	113.70
2	2	198	G	C2'-C3'-O3'	-5.02	106.17	113.70
1	1	2551	C	C1'-C2'-O2'	5.01	115.92	108.40
2	2	439	U	N1-C1'-C2'	5.01	119.51	112.00
41	i	95	GLU	CA-C-N	5.01	126.44	120.13
41	i	95	GLU	C-N-CA	5.01	126.44	120.13
52	t	27	VAL	CB-CA-C	-5.01	105.56	111.97
1	1	2481	G	C4'-C3'-O3'	-5.01	105.49	113.00
2	2	1505	G	C2'-C3'-O3'	-5.01	106.19	113.70
1	1	1138	G	C4'-C3'-O3'	-5.00	105.50	113.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	62336	0	31367	317	0
2	2	32929	0	16585	235	0
3	3	2569	0	1301	7	0
4	4	109	0	55	0	0
5	5	1622	0	830	3	0
6	6	259	0	274	9	0
7	7	2597	0	2610	94	0
8	B	2082	0	2154	33	0
9	C	1565	0	1616	23	0
10	D	1552	0	1619	13	0
11	E	1410	0	1444	16	0
12	F	1313	0	1358	9	0
13	G	1089	0	1128	7	0
14	H	980	0	1013	17	0
15	I	984	0	1035	13	0
16	J	1129	0	1162	11	0
17	K	946	0	1023	10	0
18	L	1053	0	1129	24	0
19	M	1074	0	1157	12	0
20	N	951	0	994	16	0
21	O	892	0	923	13	0
22	P	917	0	962	6	0
23	Q	947	0	1019	13	0
24	R	816	0	839	10	0
25	S	857	0	922	12	0
26	T	746	0	811	19	0
27	U	788	0	843	15	0
28	V	753	0	780	6	0
29	W	582	0	599	5	0
30	X	625	0	652	6	0
31	Y	501	0	531	10	0
32	Z	448	0	488	5	0
33	a	495	0	494	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	b	444	0	458	5	0
35	c	426	0	464	5	0
36	d	377	0	418	7	0
37	e	504	0	572	3	0
38	f	302	0	340	3	0
39	g	1760	0	1787	14	0
40	h	1636	0	1710	22	0
41	i	1643	0	1707	14	0
42	j	1152	0	1196	20	0
43	k	848	0	846	7	0
44	l	1181	0	1238	7	0
45	m	979	0	1031	6	0
46	n	1022	0	1070	16	0
47	o	790	0	831	21	0
48	p	877	0	887	9	0
49	q	957	0	1017	25	0
50	r	900	0	965	11	0
51	s	805	0	844	16	0
52	t	714	0	734	8	0
53	u	649	0	666	7	0
54	v	648	0	691	8	0
55	w	544	0	560	7	0
56	x	663	0	688	9	0
57	y	669	0	719	8	0
58	z	589	0	629	9	0
59	1	293	0	0	0	0
59	2	143	0	0	0	0
59	3	7	0	0	0	0
59	5	4	0	0	0	0
59	b	1	0	0	0	0
59	f	1	0	0	0	0
59	i	1	0	0	0	0
60	5	10	0	10	0	0
61	a	1	0	0	0	0
61	f	1	0	0	0	0
62	B	2	0	0	0	0
62	O	1	0	0	1	0
All	All	149460	0	101795	1092	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 4.

All (1092) 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)
6:6:22:ASP:CG	6:6:23:PRO:HD2	1.52	1.32
2:2:1358:U:O4	2:2:1363:A:N1	1.60	1.30
1:1:1021:A:N1	1:1:1141:U:O4	1.64	1.29
2:2:37:U:O4	2:2:397:A:N1	1.65	1.26
7:7:43:GLU:O	7:7:47:GLU:CD	1.86	1.18
2:2:1492:A:OP1	49:q:44:LYS:NZ	1.78	1.16
1:1:2314:A:OP1	11:E:88:LYS:NZ	1.77	1.16
2:2:551:U:O2'	49:q:83:ARG:NH2	1.85	1.09
1:1:2244:U:O2	1:1:2435:A:N7	1.84	1.09
7:7:45:ARG:HG3	7:7:46:LEU:HD22	1.28	1.08
2:2:563:A:N1	2:2:884:U:O4	1.87	1.06
7:7:46:LEU:HB3	7:7:61:VAL:CG2	1.86	1.06
2:2:13:U:N3	2:2:915:A:C6	2.24	1.05
2:2:13:U:N3	2:2:915:A:N6	2.03	1.05
2:2:146:G:C2'	2:2:147:G:H5'	1.87	1.03
1:1:2244:U:C2	1:1:2435:A:N7	2.31	0.99
7:7:43:GLU:O	7:7:47:GLU:OE2	1.79	0.98
2:2:481:G:O2'	2:2:483:C:N4	1.95	0.98
1:1:2297:A:N1	1:1:2321:U:C4	2.32	0.98
2:2:1060:U:C5	40:h:2:GLY:N	2.32	0.97
7:7:57:ALA:O	7:7:61:VAL:HG23	1.64	0.96
7:7:46:LEU:HD12	7:7:61:VAL:HG22	1.46	0.95
2:2:146:G:H2'	2:2:147:G:H5'	1.47	0.95
1:1:1607:C:N4	1:1:1622:G:OP2	1.99	0.95
1:1:786:C:O2'	1:1:787:C:H5'	1.65	0.94
1:1:2074:U:O4	1:1:2435:A:N6	2.01	0.94
1:1:67:U:N3	1:1:74:A:C6	2.36	0.93
1:1:2074:U:N3	1:1:2435:A:N1	2.17	0.93
1:1:2298:A:C4	1:1:2321:U:H5	1.89	0.91
6:6:22:ASP:CG	6:6:23:PRO:CD	2.42	0.91
1:1:67:U:N3	1:1:74:A:N6	2.20	0.90
2:2:13:U:C4	2:2:915:A:N6	2.39	0.90
1:1:1227:G:OP2	23:Q:16:LYS:NZ	2.03	0.90
2:2:13:U:O4	2:2:20:U:O4	1.90	0.89
1:1:2244:U:O2	1:1:2435:A:C8	2.26	0.89
7:7:46:LEU:HB3	7:7:61:VAL:CG1	2.03	0.88
1:1:1918:A:O2'	1:1:1919:A:N7	2.05	0.88
2:2:1499:A:OP2	2:2:1499:A:H3'	1.74	0.88
7:7:46:LEU:CB	7:7:61:VAL:HG13	2.04	0.87
2:2:37:U:N3	2:2:397:A:N6	2.24	0.86
2:2:827:U:H3	2:2:872:A:N6	1.74	0.86
2:2:13:U:C4	2:2:20:U:O4	2.29	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2013:A:N6	1:1:2613:U:H3	1.73	0.85
1:1:783:A:H2'	1:1:783:A:N3	1.90	0.85
7:7:46:LEU:HB3	7:7:61:VAL:HG22	1.57	0.83
1:1:2298:A:C4	1:1:2321:U:C5	2.68	0.82
12:F:121:ILE:HD12	12:F:141:ILE:HG22	1.60	0.81
42:j:111:MET:HE2	42:j:125:ALA:HB1	1.62	0.80
1:1:2000:C:OP1	20:N:5:LYS:NZ	2.15	0.80
1:1:1019:U:H3	1:1:1142:A:N6	1.78	0.79
1:1:585:G:N7	23:Q:6:ARG:NH1	2.29	0.79
2:2:1060:U:C4	40:h:2:GLY:N	2.50	0.79
7:7:46:LEU:CD1	7:7:61:VAL:HG22	2.13	0.79
18:L:58:TYR:O	37:e:13:ARG:HD3	1.83	0.79
1:1:2756:U:N3	1:1:2758:A:C6	2.52	0.78
1:1:2756:U:N3	1:1:2758:A:N6	2.31	0.78
2:2:37:U:C4	2:2:397:A:N1	2.52	0.78
2:2:915:A:N6	2:2:916:U:C4	2.53	0.77
2:2:827:U:H3	2:2:872:A:H61	1.32	0.77
7:7:45:ARG:HG3	7:7:46:LEU:CD2	2.14	0.77
7:7:45:ARG:HD2	7:7:45:ARG:O	1.86	0.76
2:2:1358:U:C4	2:2:1363:A:N1	2.53	0.76
7:7:45:ARG:CZ	7:7:51:LEU:HD21	2.15	0.76
7:7:46:LEU:HB2	7:7:61:VAL:HG13	1.66	0.75
1:1:742:A:H2'	1:1:743:A:C8	2.21	0.75
21:O:31:THR:O	21:O:102:ARG:NH1	2.20	0.75
14:H:36:ASP:O	14:H:39:THR:OG1	2.04	0.75
49:q:80:ILE:HD12	49:q:97:THR:HG22	1.70	0.74
1:1:1019:U:H3	1:1:1142:A:H61	1.35	0.74
41:i:119:SER:O	41:i:131:ASN:ND2	2.20	0.74
46:n:84:THR:HG21	46:n:103:PHE:HB3	1.70	0.74
6:6:22:ASP:OD2	6:6:23:PRO:HD2	1.88	0.74
49:q:86:ARG:HB2	49:q:86:ARG:CZ	2.17	0.74
7:7:46:LEU:CB	7:7:61:VAL:CG1	2.62	0.73
1:1:1021:A:N1	1:1:1141:U:C4	2.56	0.73
15:I:82:ALA:HB2	15:I:108:ILE:HD11	1.69	0.73
1:1:2250:G:O2'	1:1:2497:A:OP2	2.05	0.73
2:2:1218:C:H2'	2:2:1219:A:C8	2.23	0.72
7:7:42:LEU:HA	7:7:46:LEU:HD23	1.72	0.72
1:1:2297:A:N1	1:1:2321:U:O4	2.23	0.72
1:1:2445:2MG:OP1	10:D:69:ARG:NH2	2.22	0.72
2:2:439:U:O2	2:2:440:C:C6	2.42	0.72
7:7:65:ALA:HA	7:7:68:LEU:HD22	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:22:ASP:OD1	6:6:23:PRO:HD2	1.89	0.71
1:1:67:U:C4	1:1:74:A:N6	2.58	0.71
8:B:17:VAL:HB	8:B:204:VAL:HG13	1.73	0.71
1:1:954:G:OP2	19:M:16:ARG:NH2	2.23	0.70
2:2:37:U:H3	2:2:397:A:N6	1.88	0.70
53:u:4:ILE:HG12	53:u:21:VAL:HG22	1.72	0.70
2:2:972:C:O2'	47:o:57:VAL:O	2.08	0.70
7:7:42:LEU:HD21	7:7:64:GLU:HB3	1.74	0.70
51:s:47:LYS:O	51:s:50:THR:OG1	2.10	0.69
2:2:148:G:O2'	2:2:149:A:O5'	2.11	0.69
1:1:1250:G:N7	18:L:18:ARG:NH2	2.40	0.69
1:1:2885:G:N7	34:b:40:ARG:NH2	2.40	0.69
7:7:46:LEU:HB3	7:7:61:VAL:HG21	1.75	0.69
7:7:35:LYS:HB3	7:7:71:THR:HG21	1.74	0.69
1:1:1021:A:N6	1:1:1141:U:H3	1.91	0.68
56:x:49:ILE:HD12	56:x:71:LEU:HD21	1.75	0.68
1:1:2756:U:C4	1:1:2758:A:N6	2.61	0.68
35:c:17:THR:HG21	35:c:42:VAL:HB	1.75	0.68
27:U:34:VAL:HG13	27:U:67:VAL:HG22	1.74	0.68
7:7:46:LEU:CB	7:7:61:VAL:HG22	2.22	0.68
7:7:25:ALA:HB1	7:7:78:LEU:HD11	1.74	0.68
25:S:25:ARG:NH1	25:S:74:ILE:O	2.26	0.68
49:q:86:ARG:HG2	49:q:86:ARG:HH21	1.59	0.68
2:2:13:U:C2	2:2:915:A:N6	2.61	0.68
1:1:1021:A:H3'	1:1:1021:A:N3	2.08	0.67
47:o:65:TYR:HB3	51:s:96:LEU:HD11	1.75	0.67
1:1:1779:U:H5	1:1:1784:A:N7	1.91	0.67
25:S:4:ILE:HG23	25:S:106:VAL:HG22	1.76	0.67
41:i:61:VAL:HG21	41:i:200:ILE:HD11	1.76	0.67
7:7:335:LYS:HE3	7:7:342:MET:HE2	1.77	0.67
1:1:786:C:O2'	1:1:787:C:C5'	2.39	0.67
1:1:1913:A:OP2	1:1:1913:A:H3'	1.95	0.67
2:2:1060:U:C6	40:h:2:GLY:N	2.63	0.67
1:1:2013:A:N6	1:1:2613:U:N3	2.38	0.67
1:1:62:U:H2'	1:1:62:U:O2	1.95	0.66
7:7:46:LEU:HD22	7:7:46:LEU:N	2.09	0.66
1:1:1081:U:H4'	15:I:123:ALA:HB1	1.77	0.66
2:2:404:G:N7	41:i:2:ALA:HB3	2.10	0.66
1:1:2683:C:O2	17:K:70:ARG:NH2	2.28	0.66
2:2:1358:U:N3	2:2:1363:A:N6	2.43	0.66
2:2:146:G:O2'	2:2:147:G:H5'	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:658:C:H1'	52:t:22:THR:HG21	1.76	0.66
2:2:1382:C:H2'	2:2:1383:C:H5'	1.78	0.66
22:P:12:GLN:O	22:P:55:LEU:HD13	1.95	0.66
9:C:48:ILE:HG23	9:C:84:LEU:HD11	1.76	0.66
7:7:46:LEU:CG	7:7:61:VAL:HG22	2.25	0.66
2:2:1358:U:H3	2:2:1363:A:N6	1.94	0.66
1:1:2250:G:OP1	19:M:84:LYS:NZ	2.29	0.65
2:2:13:U:O4	2:2:21:G:C2	2.50	0.65
52:t:21:ASP:O	52:t:22:THR:HG22	1.96	0.65
7:7:130:ILE:HG13	7:7:183:LEU:HD23	1.78	0.65
8:B:158:ALA:O	8:B:196:GLY:O	2.14	0.65
2:2:13:U:O2	2:2:915:A:N7	2.30	0.65
2:2:1382:C:C2'	2:2:1383:C:H5'	2.26	0.65
46:n:10:GLY:HA3	46:n:78:ALA:O	1.96	0.65
1:1:807:U:P	18:L:36:LYS:NZ	2.69	0.65
1:1:1818:U:OP2	8:B:156:ARG:NH1	2.29	0.65
2:2:481:G:HO2'	2:2:483:C:H41	1.42	0.65
1:1:1082:U:N3	1:1:1086:A:N6	2.44	0.64
12:F:24:ILE:HD13	12:F:72:LEU:HD21	1.78	0.64
20:N:20:MET:HE1	20:N:40:LYS:HD3	1.79	0.64
1:1:1266:G:OP1	34:b:16:ARG:NH1	2.31	0.64
2:2:439:U:O2	2:2:440:C:C5	2.51	0.64
51:s:46:LEU:HD12	56:x:13:LEU:HD13	1.79	0.64
44:l:23:LEU:O	44:l:27:VAL:HG13	1.98	0.63
1:1:807:U:P	18:L:36:LYS:HZ1	2.22	0.63
1:1:1596:A:H2'	1:1:1597:A:C8	2.34	0.63
27:U:25:VAL:HG22	27:U:36:VAL:HG22	1.80	0.63
1:1:2685:G:OP1	17:K:78:ARG:NH2	2.31	0.63
2:2:1358:U:O4	2:2:1363:A:C2	2.47	0.63
7:7:45:ARG:NE	7:7:51:LEU:HD21	2.14	0.63
42:j:94:VAL:HG13	42:j:111:MET:HE1	1.80	0.63
26:T:2:ILE:HD13	26:T:42:GLU:HG2	1.81	0.62
1:1:572:A:OP2	24:R:80:ARG:NH2	2.32	0.62
10:D:108:ILE:HD11	10:D:180:LEU:HD13	1.80	0.62
49:q:42:PRO:HB2	49:q:89:OTD:OD1	1.99	0.62
49:q:86:ARG:HH21	49:q:86:ARG:CG	2.12	0.62
1:1:1789:A:OP2	8:B:221:ARG:NH1	2.33	0.62
1:1:927:A:H2'	1:1:928:A:C8	2.35	0.62
2:2:827:U:N3	2:2:872:A:N6	2.41	0.62
2:2:517:G:OP2	7:7:335:LYS:NZ	2.31	0.62
18:L:36:LYS:NZ	18:L:36:LYS:HB3	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:45:ARG:NH2	7:7:51:LEU:HD21	2.15	0.61
46:n:98:LEU:HB3	46:n:104:VAL:HG13	1.82	0.61
53:u:21:VAL:HG12	53:u:33:ILE:HD12	1.82	0.61
1:1:754:U:H2'	1:1:755:U:C6	2.34	0.61
2:2:1130:A:O2'	46:n:5:GLN:NE2	2.33	0.61
6:6:22:ASP:OD1	6:6:23:PRO:CD	2.46	0.61
7:7:27:GLY:O	7:7:30:PHE:HB3	2.00	0.61
15:I:27:LEU:HD13	15:I:37:PHE:CD2	2.36	0.61
12:F:35:ARG:HD3	12:F:71:LEU:HD13	1.83	0.61
9:C:156:PHE:CE1	16:J:81:ILE:HD13	2.35	0.60
1:1:1869:G:N2	1:1:1871:A:O2'	2.34	0.60
2:2:148:G:O2'	2:2:149:A:C5'	2.49	0.60
11:E:8:TYR:HA	11:E:12:VAL:HB	1.83	0.60
1:1:2245:U:O2	1:1:2435:A:C8	2.54	0.60
24:R:41:ILE:HD12	24:R:54:VAL:HG11	1.83	0.60
1:1:2376:A:N3	21:O:111:ARG:NH2	2.49	0.60
2:2:769:G:H4'	2:2:1513:A:H4'	1.84	0.60
29:W:59:LEU:HD12	29:W:80:ILE:HD12	1.84	0.60
25:S:59:GLU:HG3	25:S:66:ILE:HD11	1.84	0.60
2:2:37:U:O4	2:2:397:A:C2	2.53	0.60
2:2:966:2MG:HM22	5:5:34:C:H5''	1.82	0.60
9:C:33:ARG:NH1	9:C:53:GLY:O	2.33	0.60
1:1:1820:U:H4'	1:1:1821:A:OP2	2.00	0.60
7:7:262:VAL:HG11	7:7:284:ASN:HB3	1.82	0.60
8:B:130:LEU:HD21	8:B:192:LEU:HD23	1.84	0.60
46:n:21:ILE:HD13	46:n:63:LEU:HB3	1.84	0.60
1:1:1153:C:OP1	23:Q:92:ARG:NH1	2.35	0.60
2:2:37:U:O2	2:2:548:G:C2	2.55	0.60
2:2:945:G:C2	2:2:946:A:C8	2.90	0.59
2:2:1275:A:C2'	2:2:1276:G:H5'	2.32	0.59
14:H:23:LEU:HD12	14:H:118:ILE:HG12	1.83	0.59
7:7:45:ARG:NE	7:7:51:LEU:CD2	2.66	0.59
2:2:496:A:N3	2:2:496:A:H2'	2.17	0.59
28:V:75:GLN:HB2	28:V:92:VAL:HG23	1.83	0.59
26:T:61:LEU:HD12	26:T:61:LEU:C	2.27	0.59
48:p:107:ILE:HG21	58:z:12:PHE:CE1	2.38	0.59
1:1:1056:G:O2'	1:1:1103:A:N6	2.35	0.59
19:M:96:ILE:HG21	19:M:126:ILE:HD12	1.84	0.59
1:1:1912:A:C8	1:1:1918:A:C2	2.90	0.59
1:1:686:U:O4	36:d:12:ARG:HB2	2.03	0.59
2:2:1275:A:H2'	2:2:1276:G:H5'	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1912:A:N7	1:1:1918:A:C2	2.70	0.59
2:2:964:A:O2'	47:o:57:VAL:HG21	2.03	0.59
1:1:1406:U:O2'	1:1:1407:G:O4'	2.18	0.58
1:1:2186:G:H2'	1:1:2187:U:OP2	2.03	0.58
1:1:1047:G:HO2'	1:1:1110:G:H1	1.50	0.58
1:1:1590:A:H2'	1:1:1591:A:C8	2.38	0.58
1:1:1835:2MG:HM23	1:1:1836:C:C2	2.38	0.58
2:2:551:U:HO2'	49:q:83:ARG:NH2	1.99	0.58
15:I:78:LEU:HD22	15:I:108:ILE:HG23	1.85	0.58
31:Y:18:LEU:HB2	31:Y:53:VAL:HG11	1.85	0.58
2:2:528:C:H5''	2:2:528:C:H6	1.68	0.58
7:7:39:LEU:HB2	7:7:68:LEU:HG	1.85	0.58
39:g:187:VAL:HG21	39:g:199:VAL:HG23	1.85	0.58
1:1:1021:A:H61	1:1:1141:U:H3	1.49	0.58
12:F:50:LEU:HD13	12:F:72:LEU:HD23	1.85	0.58
1:1:984:A:N3	1:1:984:A:H2'	2.18	0.58
7:7:145:TRP:CE2	7:7:202:LEU:HB2	2.38	0.58
2:2:516:PSU:O2'	2:2:519:C:N3	2.37	0.57
42:j:56:VAL:O	42:j:60:ILE:HG23	2.02	0.57
46:n:81:HIS:O	46:n:84:THR:OG1	2.20	0.57
1:1:1421:G:C2	1:1:1422:G:C8	2.92	0.57
48:p:67:ALA:HB2	48:p:96:THR:HG23	1.86	0.57
7:7:128:ASN:HB3	7:7:185:LYS:HA	1.86	0.57
27:U:94:ARG:HB3	27:U:103:ILE:HD12	1.87	0.57
2:2:563:A:N1	2:2:884:U:C4	2.70	0.57
2:2:1061:G:H4'	47:o:58:ASN:OD1	2.04	0.57
2:2:1207:2MG:O5'	2:2:1207:2MG:H8	1.87	0.57
9:C:172:VAL:HG11	9:C:175:LEU:HD21	1.86	0.57
7:7:324:ILE:HD12	7:7:338:ARG:NH1	2.20	0.57
51:s:74:LEU:HD12	51:s:84:VAL:HG21	1.85	0.57
1:1:2436:G:O2'	1:1:2437:G:H5'	2.05	0.57
1:1:2547:A:H2'	1:1:2548:U:C6	2.40	0.57
1:1:2821:A:C2	1:1:2822:G:C4	2.92	0.57
25:S:69:LEU:HG	25:S:107:VAL:CG1	2.34	0.56
7:7:45:ARG:HD2	7:7:45:ARG:C	2.29	0.56
8:B:78:VAL:HG21	8:B:110:LEU:HD21	1.88	0.56
15:I:105:LEU:HD22	15:I:128:ILE:HG22	1.86	0.56
2:2:712:A:H2'	2:2:713:G:O4'	2.06	0.56
2:2:1356:G:H2'	2:2:1357:A:C8	2.41	0.56
7:7:46:LEU:HB3	7:7:61:VAL:CB	2.35	0.56
8:B:129:THR:C	8:B:130:LEU:HD23	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:621:A:OP2	18:L:99:ASN:ND2	2.39	0.56
7:7:46:LEU:HD12	7:7:61:VAL:CG2	2.27	0.56
1:1:1021:A:C2	1:1:1141:U:O4	2.51	0.56
1:1:1082:U:H3	1:1:1086:A:N6	2.04	0.56
2:2:216:U:H2'	2:2:217:C:C6	2.40	0.56
8:B:146:MET:HE3	8:B:154:LEU:HD21	1.87	0.56
2:2:915:A:H3'	2:2:915:A:C8	2.41	0.56
1:1:1067:A:O2'	1:1:1068:G:O4'	2.23	0.55
1:1:1993:U:H4'	9:C:133:THR:HG22	1.88	0.55
21:O:35:ILE:HG21	21:O:71:ALA:HA	1.87	0.55
2:2:1526:G:OP2	58:z:42:THR:HG23	2.07	0.55
7:7:25:ALA:HB1	7:7:78:LEU:CD1	2.36	0.55
1:1:819:A:C4	1:1:1189:A:C2	2.94	0.55
2:2:736:C:OP1	55:w:61:ARG:NH2	2.39	0.55
1:1:1095:A:O2'	1:1:1096:A:O4'	2.19	0.55
2:2:966:2MG:H5''	2:2:967:5MC:OP2	2.06	0.55
7:7:45:ARG:NE	7:7:51:LEU:HG	2.22	0.55
48:p:89:PRO:HG3	58:z:32:VAL:HG11	1.89	0.55
1:1:1109:C:O2'	1:1:1110:G:O4'	2.21	0.55
1:1:1264:A:OP1	34:b:16:ARG:NH2	2.39	0.55
49:q:85:GLY:O	49:q:94:ARG:C	2.50	0.55
1:1:2082:A:H2'	1:1:2083:G:O4'	2.07	0.55
1:1:2526:G:O2'	38:f:1:MET:HB2	2.07	0.55
2:2:1526:G:P	58:z:42:THR:HG23	2.47	0.55
17:K:38:ILE:HD11	17:K:112:PHE:HZ	1.72	0.55
1:1:2059:A:N6	1:1:2503:2MA:O2'	2.40	0.55
6:6:33:LYS:HB2	40:h:162:ILE:HD11	1.89	0.55
7:7:271:ILE:HG21	7:7:295:ARG:NH1	2.22	0.55
1:1:1914:C:C6	1:1:1915:3TD:H10A	2.42	0.55
8:B:240:PHE:O	8:B:242:LYS:N	2.39	0.55
14:H:23:LEU:HA	14:H:118:ILE:HG12	1.89	0.55
14:H:118:ILE:HB	14:H:119:PRO:HD3	1.89	0.55
21:O:7:ARG:NH1	21:O:95:SER:O	2.40	0.55
15:I:109:ALA:HB2	15:I:128:ILE:HD12	1.88	0.54
2:2:1206:G:H2'	2:2:1207:2MG:C8	2.42	0.54
7:7:26:SER:HA	7:7:29:ILE:HG23	1.89	0.54
8:B:34:LEU:CD2	8:B:63:ARG:HD3	2.38	0.54
13:G:58:LEU:O	13:G:61:VAL:HG22	2.08	0.54
1:1:1800:C:OP1	8:B:258:ARG:NH2	2.40	0.54
1:1:2244:U:C4	1:1:2435:A:N6	2.76	0.54
2:2:16:A:OP2	6:6:41:ARG:NH1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:324:ILE:HD11	7:7:325:ARG:NH2	2.22	0.54
2:2:13:U:C5	2:2:20:U:O4	2.60	0.54
2:2:481:G:HO2'	2:2:483:C:N4	2.02	0.54
20:N:28:LEU:HD23	20:N:48:VAL:HG21	1.89	0.54
26:T:10:VAL:HG12	26:T:11:LEU:HD23	1.89	0.54
43:k:49:TYR:HB3	55:w:74:HIS:CE1	2.42	0.54
7:7:42:LEU:CD2	7:7:64:GLU:HB3	2.38	0.54
57:y:35:VAL:HG11	57:y:79:LEU:HD13	1.89	0.54
1:1:1693:U:O2'	8:B:14:ARG:NH2	2.41	0.54
2:2:1308:U:P	50:r:100:GLN:HE22	2.30	0.54
11:E:42:GLU:HG3	11:E:49:LEU:HD23	1.90	0.54
27:U:36:VAL:HG11	27:U:39:ILE:HD12	1.89	0.54
2:2:429:U:O2	2:2:430:A:C8	2.61	0.53
7:7:46:LEU:HB2	7:7:61:VAL:CG1	2.36	0.53
7:7:149:LEU:HD13	7:7:219:ALA:CB	2.38	0.53
17:K:24:VAL:HG13	17:K:33:ALA:HB2	1.89	0.53
1:1:807:U:OP1	18:L:36:LYS:NZ	2.36	0.53
2:2:17:U:H2'	2:2:18:C:C6	2.43	0.53
2:2:1397:C:OP2	42:j:29:ARG:NH2	2.40	0.53
47:o:58:ASN:N	47:o:58:ASN:HD22	2.05	0.53
57:y:44:LYS:HD2	57:y:87:ALA:HB3	1.90	0.53
2:2:109:A:H2'	2:2:326:G:N2	2.23	0.53
26:T:50:LEU:HD23	31:Y:26:PHE:CE1	2.44	0.53
39:g:217:VAL:O	39:g:220:THR:HG22	2.09	0.53
2:2:629:A:H2'	2:2:630:A:O4'	2.09	0.53
2:2:1061:G:C4'	47:o:58:ASN:OD1	2.57	0.53
2:2:1112:C:N3	40:h:178:LEU:HD22	2.24	0.53
10:D:131:THR:HG22	10:D:160:ALA:O	2.09	0.53
1:1:1064:C:H2'	1:1:1065:U:C6	2.44	0.53
1:1:1656:C:OP1	9:C:141:ARG:NH1	2.41	0.53
2:2:13:U:C2	2:2:915:A:C6	2.95	0.53
42:j:99:ALA:HB3	42:j:103:THR:HG21	1.90	0.53
1:1:580:U:O3'	23:Q:31:VAL:HG13	2.08	0.53
2:2:716:A:N3	48:p:119:ASN:O	2.42	0.53
26:T:29:THR:HG23	26:T:85:VAL:O	2.09	0.53
2:2:1109:C:O4'	2:2:1109:C:C5'	2.57	0.53
2:2:1216:A:H5''	51:s:5:SER:HB3	1.91	0.53
26:T:11:LEU:HD21	26:T:46:ALA:HB3	1.90	0.53
50:r:16:VAL:HG13	50:r:34:LEU:HD12	1.90	0.53
1:1:1365:A:O5'	30:X:28:ARG:NH2	2.42	0.52
1:1:568:U:H1'	1:1:2030:6MZ:H9C1	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:S:59:GLU:CG	25:S:66:ILE:HD11	2.39	0.52
2:2:13:U:O4	2:2:20:U:C4	2.62	0.52
1:1:993:G:OP1	23:Q:50:ARG:NE	2.32	0.52
2:2:864:A:C2	2:2:865:A:C2	2.98	0.52
2:2:1175:G:N3	2:2:1176:A:C8	2.77	0.52
39:g:14:VAL:HG13	39:g:213:TYR:OH	2.10	0.52
2:2:966:2MG:H2'	2:2:966:2MG:N3	2.25	0.52
2:2:946:A:H2'	2:2:947:G:C8	2.44	0.52
19:M:30:SER:HA	19:M:133:LYS:HG2	1.92	0.52
40:h:6:HIS:HB3	51:s:89:MET:HG3	1.91	0.52
49:q:86:ARG:CB	49:q:86:ARG:NH2	2.73	0.52
1:1:870:U:OP1	19:M:6:ARG:NH1	2.43	0.52
2:2:563:A:N6	2:2:884:U:N3	2.56	0.52
40:h:77:ILE:HA	40:h:84:VAL:HG23	1.92	0.52
42:j:46:VAL:HG21	42:j:118:ALA:HB2	1.92	0.52
1:1:639:U:H2'	1:1:640:C:C6	2.45	0.52
2:2:517:G:O2'	2:2:530:G:H4'	2.10	0.52
18:L:109:LYS:HG2	18:L:126:ARG:HB2	1.92	0.52
25:S:66:ILE:HA	25:S:69:LEU:HD22	1.92	0.52
35:c:17:THR:HG21	35:c:42:VAL:CB	2.39	0.52
42:j:137:VAL:O	42:j:140:THR:OG1	2.24	0.52
49:q:42:PRO:CB	49:q:89:0TD:OD1	2.58	0.52
55:w:62:ALA:CB	55:w:68:LEU:HD12	2.40	0.52
1:1:783:A:H8	1:1:1778:U:O2'	1.92	0.52
1:1:1154:G:OP2	23:Q:58:ARG:NH1	2.42	0.52
2:2:109:A:C6	2:2:326:G:C6	2.98	0.52
2:2:531:U:OP1	7:7:214:ARG:NH1	2.42	0.52
7:7:335:LYS:CE	7:7:342:MET:HE2	2.40	0.52
18:L:74:THR:HG22	18:L:107:PHE:HB2	1.92	0.52
40:h:36:ASP:OD1	40:h:59:ARG:NH1	2.43	0.52
1:1:1020:A:C2	1:1:1141:U:C2	2.97	0.51
7:7:128:ASN:HA	7:7:189:ALA:HB3	1.92	0.51
49:q:86:ARG:CZ	49:q:86:ARG:CB	2.85	0.51
2:2:1371:G:O3'	46:n:71:GLY:HA3	2.10	0.51
18:L:36:LYS:NZ	18:L:36:LYS:CB	2.73	0.51
1:1:2788:C:H2'	1:1:2789:C:C6	2.46	0.51
20:N:55:ALA:HA	20:N:80:PHE:CE1	2.45	0.51
25:S:20:VAL:HG11	25:S:44:ALA:HA	1.90	0.51
1:1:1469:A:H2'	1:1:1470:A:C8	2.46	0.51
2:2:5:U:O2	2:2:5:U:O4'	2.27	0.51
2:2:146:G:H2'	2:2:147:G:C5'	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:325:ARG:HD3	7:7:357:LEU:HD11	1.91	0.51
40:h:51:SER:HB2	40:h:71:ALA:HB3	1.93	0.51
1:1:2006:C:O2'	1:1:2823:A:N3	2.42	0.51
2:2:421:U:O2	2:2:421:U:O4'	2.29	0.51
34:b:15:MET:O	34:b:18:SER:HB3	2.10	0.51
2:2:890:G:O2'	2:2:906:A:N6	2.44	0.51
2:2:1169:A:H2'	2:2:1170:A:C8	2.45	0.51
9:C:5:VAL:HG21	9:C:80:TRP:CD2	2.46	0.51
16:J:140:LEU:HD21	16:J:142:ILE:CD1	2.40	0.51
2:2:108:G:O6	57:y:10:ARG:HG2	2.10	0.51
2:2:1174:G:H2'	2:2:1175:G:H5'	1.92	0.51
14:H:38:MET:O	14:H:42:ARG:N	2.36	0.51
1:1:2244:U:N3	1:1:2435:A:N6	2.58	0.51
1:1:2298:A:C5	1:1:2321:U:C5	2.99	0.51
1:1:2298:A:N3	1:1:2321:U:C5	2.79	0.51
2:2:1521:C:H2'	2:2:1522:U:C6	2.46	0.51
7:7:46:LEU:CD2	7:7:46:LEU:N	2.74	0.51
46:n:130:ARG:HG3	46:n:130:ARG:HH21	1.75	0.51
2:2:107:G:N7	57:y:10:ARG:NH2	2.58	0.50
1:1:1412:U:C4	1:1:1413:A:N7	2.79	0.50
1:1:2297:A:C2	1:1:2321:U:C5	3.00	0.50
1:1:2327:A:H3'	1:1:2328:A:C8	2.46	0.50
25:S:29:VAL:HB	25:S:55:ILE:HD11	1.93	0.50
31:Y:6:LEU:HB3	31:Y:56:LEU:HD13	1.93	0.50
31:Y:42:LEU:O	31:Y:46:VAL:HG23	2.12	0.50
42:j:99:ALA:CB	42:j:103:THR:HG21	2.41	0.50
1:1:1962:5MC:H4'	1:1:1963:U:OP1	2.11	0.50
7:7:151:ARG:HA	7:7:151:ARG:NE	2.26	0.50
52:t:39:LEU:HD23	52:t:56:LEU:HB2	1.94	0.50
1:1:627:A:OP1	18:L:78:ARG:NH2	2.45	0.50
1:1:2298:A:C5	1:1:2321:U:O4	2.65	0.50
1:1:1993:U:H4'	9:C:133:THR:CG2	2.41	0.50
1:1:2502:G:H5''	1:1:2503:2MA:H5''	1.94	0.50
2:2:197:A:O2'	2:2:220:G:N2	2.44	0.50
2:2:563:A:N6	2:2:884:U:H3	2.09	0.50
2:2:657:U:O2	52:t:22:THR:HG23	2.12	0.50
2:2:1060:U:C5	40:h:2:GLY:CA	2.94	0.50
49:q:86:ARG:CG	49:q:86:ARG:NH2	2.72	0.50
57:y:55:GLN:N	57:y:56:PRO:HD2	2.27	0.50
13:G:4:ILE:HD12	13:G:18:GLN:HA	1.94	0.50
17:K:38:ILE:HD11	17:K:112:PHE:CZ	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:O:9:ARG:O	21:O:12:THR:HG22	2.11	0.50
40:h:182:ILE:HD13	40:h:203:PHE:HB2	1.93	0.50
1:1:1406:U:O2'	1:1:1407:G:O5'	2.29	0.50
1:1:2557:G:H2'	1:1:2558:C:C6	2.47	0.50
2:2:684:U:H2'	2:2:685:G:O4'	2.12	0.50
20:N:29:VAL:HG11	20:N:75:ILE:HG23	1.94	0.50
47:o:24:GLU:OE1	47:o:90:LEU:HD21	2.12	0.49
1:1:1067:A:H4'	7:7:62:SER:OG	2.11	0.49
17:K:64:ARG:NH1	17:K:102:PRO:O	2.42	0.49
27:U:13:VAL:HG22	27:U:70:VAL:HG12	1.93	0.49
57:y:44:LYS:CD	57:y:87:ALA:HB3	2.42	0.49
1:1:1827:U:OP2	8:B:221:ARG:NE	2.45	0.49
2:2:966:2MG:HM21	46:n:129:LYS:HD2	1.93	0.49
1:1:1084:A:OP1	14:H:54:VAL:HG12	2.12	0.49
1:1:2627:G:O2'	1:1:2781:A:N1	2.36	0.49
15:I:38:CYS:SG	15:I:39:LYS:N	2.85	0.49
1:1:929:U:H1'	32:Z:26:GLY:O	2.12	0.49
1:1:2196:C:O3'	1:1:2197:U:P	2.71	0.49
8:B:240:PHE:O	8:B:240:PHE:CD2	2.65	0.49
9:C:123:LYS:HE2	20:N:1:MET:HE1	1.93	0.49
39:g:111:ILE:HD12	39:g:152:LYS:HA	1.93	0.49
7:7:145:TRP:CD2	7:7:202:LEU:HB2	2.48	0.49
10:D:113:VAL:HG22	10:D:118:LEU:HD23	1.93	0.49
1:1:142:A:O2'	1:1:143:C:O4'	2.30	0.49
1:1:257:C:H2'	1:1:258:G:O4'	2.12	0.49
2:2:13:U:O4	2:2:21:G:N3	2.46	0.49
9:C:5:VAL:HG21	9:C:80:TRP:CE3	2.48	0.49
1:1:320:A:H2'	10:D:131:THR:HG21	1.95	0.49
1:1:2181:U:H2'	1:1:2182:U:O4'	2.12	0.49
2:2:961:U:O4	2:2:974:A:N1	2.45	0.49
2:2:1017:U:O2'	2:2:1018:G:O4'	2.30	0.49
26:T:11:LEU:HD21	26:T:46:ALA:CB	2.43	0.49
1:1:1007:C:OP1	16:J:37:ARG:NH2	2.45	0.49
1:1:1607:C:H4'	1:1:1608:A:O5'	2.13	0.49
9:C:2:ILE:HD13	9:C:90:PHE:CZ	2.47	0.49
10:D:21:ARG:HD2	10:D:106:LYS:HB3	1.95	0.49
39:g:80:VAL:HA	39:g:214:LEU:HD13	1.95	0.49
1:1:1282:U:H2'	1:1:1283:G:O4'	2.13	0.49
2:2:178:C:OP2	57:y:60:ARG:NH1	2.46	0.49
2:2:966:2MG:HM22	5:5:34:C:C5'	2.42	0.49
8:B:140:THR:HG22	8:B:161:TYR:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:M:30:SER:HA	19:M:133:LYS:CG	2.42	0.49
25:S:36:LEU:HD13	25:S:48:LYS:HA	1.95	0.49
29:W:53:CYS:SG	29:W:57:HIS:HA	2.53	0.49
2:2:626:G:OP1	53:u:35:ARG:NH2	2.46	0.48
11:E:123:ASP:OD1	11:E:123:ASP:C	2.55	0.48
15:I:82:ALA:CB	15:I:108:ILE:HD11	2.39	0.48
22:P:59:PHE:CE1	22:P:74:PHE:HB2	2.48	0.48
52:t:21:ASP:OD1	52:t:22:THR:N	2.42	0.48
2:2:976:G:C8	2:2:1358:U:O2	2.65	0.48
7:7:45:ARG:HE	7:7:51:LEU:HG	1.78	0.48
7:7:51:LEU:HD11	7:7:57:ALA:HB1	1.95	0.48
23:Q:58:ARG:HA	23:Q:61:TRP:CE3	2.48	0.48
54:v:75:LEU:C	54:v:75:LEU:HD12	2.38	0.48
1:1:464:U:O3'	36:d:12:ARG:NH2	2.46	0.48
1:1:2298:A:C6	1:1:2299:U:C2	3.00	0.48
1:1:2812:G:H2'	1:1:2813:A:O4'	2.12	0.48
13:G:15:LEU:HD13	13:G:15:LEU:C	2.38	0.48
27:U:13:VAL:HG23	27:U:39:ILE:HD13	1.93	0.48
1:1:74:A:N7	1:1:88:G:N7	2.60	0.48
1:1:1796:U:H2'	1:1:1797:G:C8	2.49	0.48
2:2:1111:A:C2	40:h:177:THR:HG23	2.48	0.48
1:1:785:G:H2'	1:1:786:C:C6	2.48	0.48
1:1:1664:A:H2	17:K:1:MET:HE1	1.79	0.48
1:1:2297:A:C2	1:1:2321:U:C4	2.99	0.48
7:7:45:ARG:C	7:7:45:ARG:CD	2.85	0.48
7:7:195:PRO:O	7:7:338:ARG:NH1	2.46	0.48
24:R:51:VAL:O	24:R:51:VAL:HG23	2.13	0.48
43:k:18:VAL:N	43:k:19:PRO:CD	2.77	0.48
45:m:7:ILE:HD12	45:m:36:ILE:CD1	2.43	0.48
1:1:679:C:H2'	1:1:680:C:C6	2.48	0.48
2:2:915:A:C8	2:2:915:A:C3'	2.95	0.48
54:v:20:SER:HG	54:v:71:LYS:HZ2	1.57	0.48
1:1:674:G:O2'	10:D:69:ARG:HD3	2.14	0.48
1:1:2244:U:H3	1:1:2435:A:N6	2.12	0.48
2:2:499:A:C6	2:2:547:A:C8	3.02	0.48
35:c:34:LEU:HD12	35:c:35:GLU:N	2.28	0.48
7:7:45:ARG:HE	7:7:51:LEU:CG	2.27	0.48
20:N:67:PHE:O	20:N:71:ARG:N	2.47	0.48
26:T:34:VAL:HG21	26:T:43:ILE:HD11	1.95	0.48
44:l:69:VAL:HG23	44:l:100:ALA:HB1	1.94	0.48
1:1:429:A:H2'	1:1:430:A:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1225:G:C2	1:1:1226:A:C2	3.02	0.48
1:1:2328:A:H2'	1:1:2329:U:C6	2.48	0.48
2:2:8:A:N6	41:i:206:LYS:HB2	2.29	0.48
8:B:107:PRO:HD2	8:B:110:LEU:HD22	1.96	0.48
20:N:2:ARG:HG2	20:N:2:ARG:O	2.14	0.48
41:i:48:LEU:HD21	41:i:56:ARG:HG3	1.95	0.48
1:1:784:G:H5'	1:1:785:G:OP1	2.14	0.48
1:1:1588:G:C6	1:1:1589:U:O4	2.67	0.48
1:1:1736:U:H2'	1:1:1737:G:O4'	2.14	0.48
1:1:1739:A:H2'	1:1:1740:G:O4'	2.13	0.48
7:7:191:GLY:O	7:7:362:LEU:HD11	2.14	0.48
19:M:66:ARG:NH1	19:M:104:GLU:OE1	2.47	0.48
51:s:79:LEU:HB2	51:s:84:VAL:HG22	1.96	0.48
1:1:102:U:O4	31:Y:2:LYS:N	2.47	0.47
1:1:517:C:P	34:b:10:ARG:HH22	2.36	0.47
1:1:1082:U:O2	14:H:38:MET:CG	2.61	0.47
2:2:1103:C:O2	39:g:106:THR:HG21	2.13	0.47
21:O:9:ARG:NH2	62:O:201:HOH:O	2.47	0.47
50:r:2:ALA:HB3	50:r:9:ILE:HB	1.95	0.47
2:2:1287:A:H2'	2:2:1288:A:C8	2.49	0.47
2:2:1375:A:OP1	44:l:25:LYS:NZ	2.47	0.47
7:7:262:VAL:CG1	7:7:284:ASN:HB3	2.44	0.47
11:E:74:VAL:HG22	11:E:79:ILE:HD11	1.96	0.47
1:1:2298:A:C2	1:1:2299:U:H1'	2.50	0.47
1:1:2705:A:O2'	1:1:2852:G:OP1	2.30	0.47
11:E:8:TYR:HB2	11:E:173:PHE:HZ	1.79	0.47
1:1:586:A:H5'	10:D:84:THR:HG21	1.96	0.47
1:1:2571:U:O2'	9:C:151:THR:O	2.29	0.47
2:2:526:C:OP1	49:q:88:LYS:HE3	2.13	0.47
2:2:798:U:H2'	2:2:799:G:O4'	2.14	0.47
9:C:4:LEU:HD11	9:C:100:LEU:HD22	1.95	0.47
27:U:72:ILE:HD12	27:U:83:VAL:HG21	1.96	0.47
28:V:14:LYS:O	28:V:18:ARG:HG2	2.15	0.47
42:j:13:GLU:CB	42:j:39:VAL:HG12	2.44	0.47
47:o:57:VAL:HG13	47:o:58:ASN:HD22	1.80	0.47
1:1:807:U:OP2	18:L:36:LYS:NZ	2.47	0.47
1:1:2325:G:C6	1:1:2326:C:N4	2.82	0.47
2:2:146:G:C3'	2:2:147:G:H5'	2.44	0.47
26:T:8:LEU:O	31:Y:29:ARG:NH1	2.47	0.47
43:k:51:ILE:HG13	43:k:85:ILE:HG21	1.97	0.47
45:m:121:LEU:HD12	45:m:121:LEU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:25:THR:HG21	9:C:193:VAL:HG22	1.96	0.47
11:E:171:ALA:O	11:E:174:ASP:N	2.48	0.47
20:N:44:LEU:O	20:N:45:ARG:C	2.58	0.47
46:n:55:VAL:HG23	46:n:55:VAL:O	2.14	0.47
50:r:71:ARG:HB2	50:r:71:ARG:CZ	2.43	0.47
1:1:706:A:H2'	1:1:707:G:O4'	2.14	0.47
1:1:1230:A:H2'	1:1:1231:U:O4'	2.14	0.47
2:2:881:G:OP2	49:q:9:ARG:NH1	2.48	0.47
2:2:1316:G:N2	2:2:1318:A:H3'	2.30	0.47
9:C:26:VAL:HG22	9:C:188:LEU:HD22	1.96	0.47
24:R:68:ARG:HD3	24:R:92:TRP:CZ2	2.50	0.47
26:T:8:LEU:HD13	31:Y:22:LEU:HB3	1.96	0.47
35:c:10:LYS:HD2	35:c:20:PHE:CD2	2.49	0.47
41:i:61:VAL:HA	41:i:64:ILE:HD12	1.96	0.47
42:j:81:LEU:HD13	42:j:123:VAL:CG1	2.45	0.47
56:x:51:VAL:HG21	56:x:71:LEU:HD22	1.95	0.47
1:1:742:A:C2	1:1:743:A:C6	3.03	0.47
2:2:309:A:O2'	2:2:607:A:N1	2.46	0.47
26:T:50:LEU:HD23	31:Y:26:PHE:CZ	2.49	0.47
56:x:36:ARG:NH2	56:x:75:ALA:O	2.48	0.47
7:7:240:LEU:HD21	7:7:264:VAL:HG13	1.97	0.47
1:1:1980:G:O2'	1:1:1982:U:OP2	2.32	0.47
7:7:39:LEU:HA	7:7:68:LEU:HD21	1.96	0.47
7:7:45:ARG:NE	7:7:51:LEU:CG	2.78	0.47
26:T:7:LEU:HD22	26:T:46:ALA:HA	1.97	0.47
39:g:129:LEU:HD13	39:g:134:ALA:CB	2.44	0.47
2:2:1516:2MG:N2	2:2:1519:MA6:OP2	2.49	0.46
16:J:41:LYS:NZ	16:J:50:THR:O	2.48	0.46
46:n:55:VAL:O	46:n:57:MET:N	2.47	0.46
1:1:1338:G:C6	1:1:1339:G:C5	3.03	0.46
1:1:2602:A:H5''	1:1:2603:G:H5''	1.97	0.46
1:1:2313:C:H5''	11:E:88:LYS:HD2	1.98	0.46
1:1:2409:G:H2'	1:1:2410:G:O4'	2.15	0.46
2:2:195:A:H2'	2:2:196:A:C8	2.50	0.46
11:E:8:TYR:HB2	11:E:173:PHE:CZ	2.50	0.46
18:L:36:LYS:HB3	18:L:36:LYS:HZ3	1.80	0.46
26:T:58:VAL:HG22	26:T:85:VAL:HG13	1.97	0.46
1:1:572:A:C2	1:1:2033:A:C2	3.03	0.46
1:1:2056:G:H2'	1:1:2056:G:N3	2.29	0.46
2:2:13:U:C4	2:2:21:G:C2	3.03	0.46
2:2:515:G:H2'	2:2:516:PSU:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:567:G:H2'	2:2:568:G:O4'	2.16	0.46
16:J:112:GLY:O	16:J:115:GLY:N	2.48	0.46
1:1:1962:5MC:O2'	1:1:1964:G:OP2	2.32	0.46
2:2:50:A:O2'	2:2:360:G:N2	2.48	0.46
2:2:1227:A:C8	50:r:116:ILE:HD12	2.50	0.46
2:2:1288:A:N3	2:2:1352:C:O2'	2.48	0.46
2:2:1499:A:H3'	2:2:1499:A:P	2.55	0.46
19:M:82:MET:HA	19:M:82:MET:HE2	1.98	0.46
1:1:53:A:H2'	1:1:54:G:O4'	2.15	0.46
1:1:1125:G:C6	1:1:1126:A:N6	2.84	0.46
7:7:165:GLU:CG	7:7:277:THR:HG21	2.46	0.46
8:B:260:ASN:OD1	8:B:263:THR:N	2.48	0.46
17:K:7:MET:HE2	17:K:44:LYS:CG	2.46	0.46
27:U:27:ASN:OD1	27:U:27:ASN:C	2.59	0.46
42:j:107:ALA:HB2	42:j:125:ALA:HB3	1.97	0.46
55:w:12:ARG:O	55:w:16:GLU:HG3	2.15	0.46
58:z:4:ILE:HD12	58:z:19:PHE:HA	1.98	0.46
1:1:2585:U:O2	1:1:2585:U:O4'	2.33	0.46
2:2:956:U:H2'	2:2:957:U:O4'	2.15	0.46
2:2:198:G:H2'	2:2:199:A:H8	1.79	0.46
9:C:175:LEU:CD1	9:C:193:VAL:HG12	2.46	0.46
20:N:38:LEU:N	20:N:39:PRO:CD	2.79	0.46
22:P:10:GLN:HE21	22:P:10:GLN:HA	1.81	0.46
40:h:113:ALA:HA	40:h:202:ILE:HD12	1.97	0.46
2:2:376:G:C2	2:2:389:A:C2	3.03	0.46
11:E:79:ILE:HG21	11:E:85:ILE:HD13	1.97	0.46
1:1:729:G:H2'	1:1:1775:U:H1'	1.98	0.46
1:1:1779:U:C5	1:1:1784:A:N7	2.79	0.46
1:1:2298:A:C2	1:1:2321:U:C5	3.04	0.46
2:2:501:C:H1'	2:2:549:C:H1'	1.97	0.46
7:7:42:LEU:CG	7:7:64:GLU:HB3	2.46	0.46
7:7:45:ARG:O	7:7:51:LEU:HG	2.16	0.46
11:E:93:GLY:O	11:E:96:MET:HB3	2.15	0.46
43:k:66:ALA:HB1	43:k:67:PRO:HD2	1.97	0.46
46:n:84:THR:HG21	46:n:103:PHE:CB	2.43	0.46
54:v:17:MET:HE3	54:v:20:SER:HB3	1.97	0.46
1:1:191:A:H2'	1:1:192:C:C6	2.51	0.45
1:1:1433:A:H2'	1:1:1434:A:O4'	2.17	0.45
2:2:429:U:N3	2:2:431:A:N6	2.63	0.45
7:7:39:LEU:HD13	7:7:68:LEU:HD23	1.98	0.45
18:L:76:GLU:HB2	18:L:111:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:M:65:ILE:HG23	19:M:103:TYR:CE1	2.51	0.45
1:1:2715:C:C4	1:1:2716:C:C5	3.05	0.45
9:C:2:ILE:HD12	9:C:48:ILE:HD11	1.99	0.45
26:T:51:PHE:CD2	26:T:93:LEU:HD12	2.51	0.45
38:f:11:CYS:SG	38:f:33:HIS:CG	3.10	0.45
47:o:6:ILE:HD12	47:o:84:VAL:HG22	1.98	0.45
1:1:332:A:C2	1:1:335:C:C5	3.04	0.45
1:1:783:A:N3	1:1:783:A:C2'	2.71	0.45
2:2:22:G:C6	2:2:23:C:C4	3.04	0.45
8:B:144:VAL:HB	8:B:154:LEU:HB2	1.98	0.45
13:G:5:LEU:C	13:G:6:LEU:HD23	2.41	0.45
31:Y:26:PHE:CE1	31:Y:30:MET:HE3	2.52	0.45
1:1:644:A:H2'	1:1:645:C:O4'	2.15	0.45
1:1:2455:G:H2'	1:1:2456:C:C6	2.52	0.45
2:2:1188:A:O3'	51:s:98:LYS:NZ	2.50	0.45
8:B:76:ALA:HB3	8:B:116:ILE:HG13	1.99	0.45
17:K:7:MET:HE2	17:K:44:LYS:HG3	1.97	0.45
39:g:187:VAL:CG2	39:g:199:VAL:HG23	2.46	0.45
53:u:21:VAL:HG21	53:u:60:TRP:CD1	2.52	0.45
1:1:523:C:H4'	1:1:540:C:O2	2.16	0.45
8:B:142:HIS:ND1	8:B:193:GLY:O	2.48	0.45
22:P:106:LYS:O	22:P:109:ARG:NH2	2.43	0.45
46:n:44:ALA:O	46:n:47:VAL:HG22	2.16	0.45
1:1:615:U:O4	10:D:39:ALA:HB2	2.17	0.45
1:1:1385:A:C4	1:1:1403:A:C2	3.05	0.45
1:1:1789:A:OP1	8:B:221:ARG:HG3	2.17	0.45
1:1:2071:A:H2'	1:1:2072:C:C6	2.52	0.45
1:1:2107:G:C6	1:1:2183:A:C2	3.04	0.45
1:1:2816:G:N3	1:1:2883:A:O2'	2.40	0.45
2:2:13:U:O4	2:2:21:G:C4	2.69	0.45
2:2:108:G:C6	57:y:10:ARG:HG2	2.51	0.45
2:2:1064:G:O2'	2:2:1190:G:N2	2.50	0.45
2:2:1255:G:O2'	2:2:1258:G:N3	2.43	0.45
23:Q:85:LYS:HB3	23:Q:116:ALA:HB1	1.98	0.45
25:S:74:ILE:HD12	25:S:105:VAL:CG2	2.47	0.45
35:c:23:THR:OG1	35:c:24:THR:N	2.49	0.45
40:h:35:SER:HG	40:h:59:ARG:HH12	1.61	0.45
47:o:92:LEU:HD22	47:o:98:VAL:HG13	1.98	0.45
48:p:18:ASP:HB3	48:p:81:ASN:HB2	1.99	0.45
54:v:79:VAL:HG22	54:v:80:GLU:HG3	1.98	0.45
56:x:15:LEU:HD13	56:x:33:THR:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:372:G:C8	30:X:61:LYS:HD2	2.51	0.45
1:1:783:A:H8	1:1:1778:U:HO2'	1.61	0.45
1:1:910:A:N3	1:1:2264:C:O2'	2.48	0.45
2:2:842:U:H3'	2:2:843:U:C5'	2.46	0.45
2:2:1518:MA6:H103	2:2:1519:MA6:N6	2.32	0.45
19:M:21:ALA:HB1	19:M:100:LYS:HG2	1.98	0.45
20:N:63:ARG:HA	20:N:80:PHE:CE2	2.52	0.45
26:T:2:ILE:HG21	26:T:7:LEU:HD21	1.97	0.45
45:m:106:THR:HB	45:m:121:LEU:HD13	1.99	0.45
54:v:61:ILE:HA	54:v:75:LEU:HA	1.99	0.45
1:1:67:U:C2	1:1:74:A:N6	2.85	0.45
1:1:587:C:OP2	18:L:21:ARG:NH1	2.50	0.45
1:1:1968:G:O2'	1:1:1969:A:O4'	2.28	0.45
2:2:337:G:H2'	2:2:338:A:C8	2.51	0.45
2:2:757:U:OP1	2:2:822:U:O2'	2.33	0.45
2:2:1359:C:OP2	51:s:75:ARG:NE	2.48	0.45
7:7:45:ARG:HD2	7:7:51:LEU:HG	1.99	0.45
21:O:53:THR:HG23	21:O:74:VAL:HG21	1.99	0.45
42:j:56:VAL:N	42:j:57:PRO:CD	2.80	0.45
58:z:58:LYS:O	58:z:62:ARG:HG2	2.17	0.45
1:1:1425:G:H2'	1:1:1426:G:O4'	2.17	0.45
1:1:1853:A:N1	1:1:2087:G:H1'	2.32	0.45
2:2:622:A:C8	2:2:623:C:C6	3.05	0.45
9:C:62:LYS:HB2	9:C:63:PRO:HD3	1.99	0.45
1:1:271:G:O2'	1:1:272:A:O5'	2.34	0.45
1:1:1783:A:N1	1:1:2587:A:H2'	2.32	0.45
2:2:36:C:O2'	49:q:114:ARG:NH2	2.50	0.45
2:2:1176:A:H2'	2:2:1177:G:O4'	2.17	0.45
11:E:121:SER:O	11:E:121:SER:OG	2.32	0.45
16:J:84:ILE:HG23	16:J:84:ILE:O	2.17	0.45
21:O:27:VAL:HG21	21:O:40:ILE:HD12	1.99	0.45
21:O:53:THR:HG23	21:O:74:VAL:CG2	2.47	0.45
23:Q:88:VAL:HG22	24:R:51:VAL:HG12	1.98	0.45
33:a:60:PHE:CE2	56:x:42:PRO:HD3	2.52	0.45
40:h:177:THR:HG22	40:h:179:ARG:HG2	1.98	0.45
54:v:48:ASP:HB3	54:v:75:LEU:HD23	2.00	0.45
1:1:833:A:H2'	1:1:834:G:C8	2.52	0.44
41:i:48:LEU:HD23	41:i:53:VAL:HG12	1.97	0.44
46:n:47:VAL:CG2	46:n:76:ALA:HB1	2.47	0.44
56:x:51:VAL:CG2	56:x:71:LEU:HD22	2.47	0.44
2:2:371:A:H2'	2:2:372:C:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1320:C:O2	56:x:36:ARG:NH1	2.50	0.44
7:7:42:LEU:HD23	7:7:68:LEU:HD21	2.00	0.44
40:h:121:THR:HG23	40:h:189:ALA:HA	2.00	0.44
49:q:33:VAL:HG22	49:q:79:VAL:HG22	1.98	0.44
2:2:767:A:H2'	2:2:768:A:O4'	2.17	0.44
3:3:78:A:C2	3:3:99:A:C4	3.05	0.44
10:D:103:GLY:HA2	10:D:106:LYS:HD3	2.00	0.44
20:N:49:GLU:HB2	20:N:50:PRO:HD3	1.99	0.44
24:R:21:ARG:O	24:R:22:LEU:HD23	2.17	0.44
40:h:134:MET:HE2	40:h:168:TYR:CD2	2.52	0.44
45:m:7:ILE:HD12	45:m:36:ILE:HD12	1.99	0.44
1:1:117:G:C6	1:1:119:A:N6	2.85	0.44
1:1:693:A:H2'	1:1:694:U:O4'	2.17	0.44
1:1:1283:G:H1'	1:1:1329:U:O2	2.17	0.44
1:1:1923:U:O2'	1:1:1924:C:C6	2.69	0.44
2:2:35:G:N3	49:q:115:SER:OG	2.49	0.44
2:2:339:C:OP2	17:K:98:ARG:NH1	2.51	0.44
22:P:32:VAL:HG21	22:P:41:GLN:HB2	2.00	0.44
26:T:39:THR:HG22	26:T:42:GLU:CD	2.42	0.44
49:q:10:LYS:O	49:q:10:LYS:HG3	2.17	0.44
50:r:4:ILE:CG1	50:r:9:ILE:HD12	2.48	0.44
53:u:63:GLN:OE1	53:u:63:GLN:HA	2.18	0.44
1:1:117:G:C6	1:1:119:A:C6	3.06	0.44
1:1:396:G:OP2	30:X:10:LYS:NZ	2.50	0.44
1:1:2133:G:O2'	1:1:2157:G:N2	2.51	0.44
1:1:2469:A:N6	1:1:2481:G:O2'	2.51	0.44
2:2:865:A:H2'	2:2:866:C:C6	2.53	0.44
27:U:34:VAL:HG23	27:U:36:VAL:HG23	1.99	0.44
51:s:67:THR:HG21	51:s:83:LYS:HE2	2.00	0.44
1:1:125:A:OP2	36:d:19:ARG:NH2	2.49	0.44
1:1:922:C:H1'	29:W:26:PHE:HD2	1.81	0.44
1:1:1779:U:O2	1:1:1783:A:C6	2.71	0.44
1:1:2805:C:H2'	1:1:2806:C:O4'	2.17	0.44
2:2:135:C:N3	53:u:1:MET:N	2.66	0.44
2:2:384:G:H2'	2:2:385:C:C6	2.52	0.44
2:2:502:A:H2'	2:2:503:C:O4'	2.17	0.44
3:3:24:G:N7	3:3:56:G:H2'	2.33	0.44
18:L:36:LYS:HB3	18:L:36:LYS:HZ2	1.83	0.44
28:V:77:VAL:CG2	28:V:86:LEU:HD22	2.48	0.44
1:1:1182:G:H2'	1:1:1183:U:O4'	2.17	0.44
1:1:1681:G:N3	1:1:1762:A:H2'	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2500:U:O2	1:1:2504:PSU:C2	2.70	0.44
2:2:401:C:O2'	2:2:621:A:N3	2.41	0.44
2:2:1111:A:N1	40:h:177:THR:HG23	2.33	0.44
2:2:1435:G:H2'	2:2:1436:U:C6	2.52	0.44
46:n:25:ASN:OD1	46:n:25:ASN:N	2.49	0.44
1:1:566:U:O4	24:R:80:ARG:HD3	2.18	0.44
1:1:782:A:C6	8:B:225:MET:HE2	2.53	0.44
2:2:495:A:C6	2:2:496:A:N6	2.86	0.44
9:C:142:VAL:HB	9:C:143:PRO:HD2	2.00	0.44
13:G:47:PHE:HA	13:G:51:ARG:HB2	2.00	0.44
25:S:17:VAL:HG12	25:S:76:VAL:HG21	2.00	0.44
42:j:13:GLU:HB2	42:j:39:VAL:HG12	2.00	0.44
55:w:41:PRO:HD2	55:w:44:ILE:HD12	2.00	0.44
2:2:13:U:C4	2:2:915:A:C6	2.98	0.44
2:2:323:U:H2'	2:2:324:G:O4'	2.18	0.44
2:2:397:A:H3'	2:2:397:A:N3	2.33	0.44
26:T:2:ILE:HD11	26:T:6:ARG:CG	2.46	0.44
39:g:129:LEU:HD13	39:g:134:ALA:HB2	1.99	0.44
1:1:46:G:C6	1:1:47:C:C4	3.06	0.43
1:1:201:C:OP1	30:X:18:ARG:NH1	2.50	0.43
1:1:820:A:H2'	1:1:821:A:O4'	2.18	0.43
1:1:2242:G:H2'	1:1:2243:U:O4'	2.18	0.43
1:1:2680:U:H5'	9:C:194:PRO:HA	1.99	0.43
2:2:1275:A:C3'	2:2:1276:G:H5'	2.48	0.43
6:6:23:PRO:O	6:6:24:LEU:C	2.61	0.43
7:7:194:SER:N	7:7:195:PRO:HD2	2.33	0.43
18:L:82:LEU:HD22	18:L:90:VAL:HG21	2.00	0.43
1:1:964:C:O2'	1:1:2273:A:N3	2.39	0.43
1:1:1149:G:H2'	1:1:1150:C:C6	2.53	0.43
1:1:2646:C:O5'	1:1:2646:C:H6	2.00	0.43
1:1:2803:G:H2'	1:1:2804:U:C6	2.53	0.43
2:2:346:G:OP1	22:P:39:ARG:NH2	2.44	0.43
9:C:149:ASN:O	9:C:151:THR:N	2.50	0.43
11:E:59:ALA:O	33:a:27:THR:OG1	2.35	0.43
14:H:118:ILE:N	14:H:118:ILE:HD12	2.33	0.43
26:T:6:ARG:O	26:T:10:VAL:HG23	2.18	0.43
50:r:16:VAL:HG13	50:r:34:LEU:CD1	2.48	0.43
1:1:1059:G:N3	15:I:127:SER:OG	2.51	0.43
1:1:1250:G:OP2	18:L:21:ARG:NH2	2.51	0.43
1:1:2395:C:H2'	1:1:2396:G:O4'	2.18	0.43
1:1:2758:A:H2'	1:1:2759:G:O4'	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2898:U:O2'	16:J:134:ALA:O	2.26	0.43
13:G:99:ILE:O	13:G:103:VAL:HG23	2.19	0.43
47:o:65:TYR:HB3	51:s:96:LEU:CD1	2.47	0.43
1:1:811:U:H2'	18:L:21:ARG:HA	2.00	0.43
1:1:1370:C:H2'	1:1:1371:G:O4'	2.18	0.43
1:1:1783:A:C2	1:1:2587:A:C4	3.07	0.43
1:1:2194:U:H2'	1:1:2195:U:O4'	2.18	0.43
2:2:938:A:N6	2:2:939:G:C6	2.87	0.43
7:7:38:ARG:O	7:7:42:LEU:HD22	2.18	0.43
7:7:350:LEU:O	7:7:351:ASP:C	2.60	0.43
41:i:203:LEU:O	41:i:206:LYS:HB3	2.18	0.43
47:o:21:ALA:HB1	47:o:92:LEU:HD23	2.01	0.43
1:1:414:C:H2'	1:1:415:A:C8	2.54	0.43
1:1:2902:C:H2'	1:1:2903:U:H5'	2.00	0.43
2:2:37:U:N3	2:2:397:A:C6	2.87	0.43
2:2:826:C:O2	45:m:16:ASN:ND2	2.52	0.43
27:U:14:LEU:HD11	27:U:71:ALA:HB2	2.01	0.43
37:e:27:ALA:O	37:e:28:ASN:HB2	2.18	0.43
50:r:3:ARG:HA	50:r:7:ILE:O	2.18	0.43
53:u:6:LEU:HG	53:u:17:TYR:HB3	2.00	0.43
1:1:554:U:O4	1:1:555:G:C6	2.71	0.43
1:1:1038:G:H2'	1:1:1039:A:C8	2.53	0.43
1:1:1246:A:H2'	1:1:1247:A:O4'	2.18	0.43
1:1:1939:5MU:OP1	1:1:2604:U:O2'	2.37	0.43
2:2:171:A:H2'	2:2:172:A:C8	2.53	0.43
2:2:1389:C:H2'	2:2:1390:U:O4'	2.19	0.43
2:2:1518:MA6:N6	2:2:1519:MA6:H93	2.32	0.43
16:J:140:LEU:HD21	16:J:142:ILE:HD12	2.01	0.43
21:O:51:ALA:HB3	21:O:78:VAL:HB	2.01	0.43
21:O:75:GLY:O	21:O:78:VAL:HG12	2.19	0.43
30:X:7:VAL:HG21	30:X:59:ILE:HD11	2.00	0.43
2:2:13:U:C2	2:2:915:A:C5	3.07	0.43
18:L:101:ILE:HD12	18:L:105:ILE:HG21	2.00	0.43
1:1:799:G:C6	1:1:800:A:C6	3.07	0.43
1:1:879:G:H2'	1:1:880:G:O4'	2.19	0.43
7:7:42:LEU:HD11	7:7:64:GLU:HB3	2.00	0.43
9:C:159:LYS:HG2	9:C:161:MET:HE3	2.01	0.43
14:H:123:ILE:HD13	14:H:123:ILE:O	2.19	0.43
27:U:13:VAL:CG2	27:U:39:ILE:HD13	2.49	0.43
43:k:96:VAL:HG23	43:k:96:VAL:O	2.18	0.43
1:1:947:A:H2'	1:1:948:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1095:A:C4	7:7:52:TRP:CE3	3.07	0.43
1:1:1912:A:N1	2:2:1407:5MC:O2'	2.46	0.43
2:2:264:C:H2'	2:2:265:G:O4'	2.19	0.43
2:2:1309:G:N7	50:r:98:ARG:NH2	2.67	0.43
7:7:287:LEU:O	7:7:290:LYS:HG2	2.19	0.43
39:g:61:ALA:HB3	39:g:224:GLY:HA3	2.00	0.43
1:1:1779:U:O2	1:1:1783:A:N6	2.52	0.43
7:7:165:GLU:HG3	7:7:277:THR:HG21	2.00	0.43
20:N:12:ARG:NE	20:N:20:MET:HE3	2.33	0.43
1:1:460:A:H2'	1:1:461:C:O4'	2.18	0.42
1:1:548:G:H3'	1:1:549:G:O4'	2.19	0.42
2:2:620:C:H2'	2:2:621:A:O4'	2.19	0.42
7:7:49:PRO:HA	7:7:52:TRP:HB2	2.01	0.42
8:B:245:VAL:HA	8:B:250:VAL:O	2.19	0.42
27:U:36:VAL:CG1	27:U:39:ILE:HD12	2.49	0.42
39:g:28:LYS:N	39:g:29:PRO:CD	2.82	0.42
41:i:140:ASN:N	41:i:182:PHE:O	2.48	0.42
1:1:319:G:H2'	1:1:320:A:O4'	2.19	0.42
1:1:871:U:H2'	1:1:872:U:C6	2.55	0.42
1:1:2474:U:H2'	1:1:2475:C:C6	2.54	0.42
1:1:2803:G:H2'	1:1:2804:U:C5	2.54	0.42
2:2:928:G:O2'	2:2:929:G:H5'	2.19	0.42
7:7:99:ALA:O	7:7:103:GLU:N	2.51	0.42
7:7:131:LEU:HB3	7:7:223:VAL:HG13	2.00	0.42
12:F:137:ASP:O	12:F:141:ILE:HG23	2.19	0.42
14:H:23:LEU:HD23	14:H:87:GLU:CD	2.44	0.42
26:T:11:LEU:HD23	26:T:11:LEU:N	2.34	0.42
46:n:19:VAL:HG11	46:n:83:ILE:HA	2.01	0.42
47:o:22:THR:HG23	47:o:74:VAL:HG21	2.02	0.42
52:t:35:GLN:NE2	52:t:39:LEU:HD13	2.34	0.42
1:1:122:G:H2'	1:1:123:G:O4'	2.20	0.42
1:1:1401:G:C6	1:1:1402:U:C4	3.06	0.42
2:2:1530:G:H2'	2:2:1531:A:C8	2.54	0.42
3:3:61:G:C6	3:3:62:C:C4	3.08	0.42
11:E:29:PRO:HB2	11:E:169:LEU:HD22	2.00	0.42
29:W:37:ILE:HD11	29:W:82:ILE:HD11	2.01	0.42
32:Z:7:ILE:HD11	32:Z:48:ILE:HD11	2.01	0.42
1:1:1130:U:C4	9:C:152:PRO:HA	2.54	0.42
1:1:1562:U:H2'	1:1:1563:U:O4'	2.19	0.42
1:1:2026:U:C2'	1:1:2027:G:O5'	2.67	0.42
2:2:921:U:O2'	42:j:24:THR:O	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:324:ILE:HG12	7:7:325:ARG:N	2.34	0.42
8:B:205:LEU:HG	8:B:210:ALA:HB1	2.01	0.42
14:H:121:SER:OG	14:H:126:LEU:HD11	2.19	0.42
24:R:63:VAL:HG13	24:R:94:THR:HG23	2.02	0.42
27:U:5:ILE:CD1	27:U:70:VAL:HG23	2.48	0.42
52:t:57:LEU:HD23	52:t:57:LEU:HA	1.93	0.42
1:1:1804:C:OP1	8:B:257:THR:HG22	2.20	0.42
2:2:254:G:O2'	54:v:18:GLU:O	2.37	0.42
2:2:502:A:C2	2:2:544:G:C2	3.07	0.42
2:2:1328:C:H2'	2:2:1329:A:O4'	2.19	0.42
7:7:162:PHE:HB3	7:7:184:VAL:CG2	2.50	0.42
14:H:23:LEU:HD13	14:H:92:ALA:HA	2.01	0.42
20:N:49:GLU:N	20:N:50:PRO:CD	2.82	0.42
30:X:7:VAL:HA	30:X:71:LEU:HD21	2.01	0.42
41:i:55:LEU:O	41:i:59:GLN:HG2	2.19	0.42
47:o:90:LEU:HD22	47:o:91:ASP:N	2.34	0.42
49:q:55:VAL:HG21	49:q:80:ILE:HD11	2.01	0.42
1:1:2756:U:C4	1:1:2759:G:C6	3.07	0.42
1:1:2758:A:O4'	12:F:64:GLN:NE2	2.46	0.42
2:2:1403:C:H6	2:2:1403:C:O5'	2.03	0.42
44:l:30:LEU:HD11	44:l:116:MET:HE2	2.00	0.42
44:l:93:PRO:HA	44:l:96:ARG:HD3	2.01	0.42
1:1:62:U:O2	1:1:62:U:C2'	2.66	0.42
1:1:324:A:H2'	1:1:325:G:O4'	2.20	0.42
1:1:807:U:P	18:L:36:LYS:HZ3	2.41	0.42
2:2:1126:U:O2	2:2:1280:A:H5'	2.19	0.42
3:3:29:A:C2	3:3:56:G:C2	3.07	0.42
28:V:30:ILE:HD11	28:V:63:ILE:HG21	2.02	0.42
39:g:188:ASP:OD1	39:g:189:THR:N	2.52	0.42
47:o:22:THR:O	47:o:25:ILE:HG22	2.19	0.42
49:q:23:ALA:HB1	49:q:57:LEU:HD12	2.02	0.42
52:t:67:LEU:HD21	52:t:87:LEU:HD13	2.01	0.42
55:w:71:THR:OG1	55:w:72:ASP:N	2.52	0.42
1:1:848:C:H2'	1:1:849:A:C8	2.55	0.42
1:1:2315:G:O2'	1:1:2316:G:O4'	2.37	0.42
2:2:110:C:N4	2:2:111:G:C6	2.88	0.42
7:7:149:LEU:HD13	7:7:219:ALA:HB3	2.01	0.42
8:B:82:GLU:HB2	8:B:91:ILE:HG13	2.02	0.42
12:F:52:PHE:CE2	12:F:69:ARG:HA	2.54	0.42
14:H:23:LEU:HD12	14:H:118:ILE:CG1	2.49	0.42
1:1:1027:A:C6	1:1:1126:A:C4	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1169:A:N3	1:1:1169:A:H5''	2.35	0.42
1:1:1245:G:OP1	18:L:13:LYS:NZ	2.52	0.42
1:1:1327:A:H2'	1:1:1328:A:O4'	2.19	0.42
1:1:1796:U:H2'	1:1:1797:G:H8	1.84	0.42
2:2:496:A:N3	2:2:496:A:C2'	2.82	0.42
2:2:860:A:H2'	2:2:861:G:O4'	2.20	0.42
2:2:1251:A:H2'	2:2:1252:A:O4'	2.20	0.42
3:3:106:G:H2'	3:3:107:G:O4'	2.20	0.42
7:7:46:LEU:HB3	7:7:61:VAL:HG11	1.94	0.42
20:N:38:LEU:HB3	20:N:39:PRO:HD3	2.02	0.42
28:V:51:GLN:HG2	28:V:86:LEU:HD11	2.02	0.42
31:Y:14:LEU:HD23	31:Y:14:LEU:HA	1.86	0.42
33:a:36:VAL:C	33:a:37:CYS:SG	2.97	0.42
42:j:15:LEU:HD12	42:j:15:LEU:C	2.44	0.42
43:k:88:MET:HB2	55:w:65:LEU:HD21	2.00	0.42
58:z:4:ILE:HD12	58:z:19:PHE:CA	2.50	0.42
1:1:1021:A:N3	1:1:1021:A:C3'	2.79	0.42
1:1:1323:C:OP1	25:S:98:LYS:HD2	2.20	0.42
1:1:1923:U:O2'	1:1:1924:C:H6	2.01	0.42
2:2:857:C:H2'	2:2:858:G:O4'	2.20	0.42
2:2:1241:G:OP1	44:l:35:LYS:NZ	2.52	0.42
6:6:22:ASP:CB	6:6:23:PRO:HD2	2.34	0.42
7:7:31:ASP:OD1	7:7:31:ASP:N	2.52	0.42
16:J:28:LEU:O	16:J:32:LEU:HG	2.20	0.42
18:L:4:ASN:C	18:L:4:ASN:HD22	2.28	0.42
39:g:114:LEU:HD13	39:g:144:LEU:CB	2.50	0.42
40:h:112:ASP:HB3	40:h:115:LEU:HD12	2.02	0.42
1:1:685:A:H5''	1:1:788:A:H62	1.85	0.41
1:1:1916:A:H2'	1:1:1917:PSU:C6	2.54	0.41
2:2:8:A:C6	41:i:206:LYS:HB2	2.55	0.41
2:2:61:G:H2'	2:2:62:U:O4'	2.20	0.41
2:2:559:A:H4'	2:2:560:A:H3'	2.02	0.41
2:2:1231:G:C6	2:2:1232:U:C4	3.08	0.41
2:2:1377:A:O2'	44:l:2:PRO:HG3	2.19	0.41
19:M:41:LEU:HD21	19:M:126:ILE:HD13	2.00	0.41
48:p:31:ILE:HG12	48:p:46:THR:HG22	2.01	0.41
50:r:16:VAL:O	50:r:20:THR:HG23	2.20	0.41
1:1:289:G:H2'	1:1:290:U:O4'	2.20	0.41
1:1:981:A:N1	1:1:2027:G:O2'	2.43	0.41
1:1:1019:U:N3	1:1:1142:A:N6	2.48	0.41
1:1:1073:A:N6	1:1:1074:G:C6	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:872:A:N3	2:2:872:A:H2'	2.36	0.41
2:2:1125:U:OP1	47:o:37:ARG:HD2	2.20	0.41
7:7:45:ARG:CD	7:7:51:LEU:HG	2.50	0.41
7:7:133:ILE:HD11	7:7:153:TYR:HD2	1.84	0.41
11:E:60:ILE:O	11:E:102:ARG:NH2	2.53	0.41
14:H:23:LEU:HD22	14:H:93:ALA:N	2.35	0.41
23:Q:65:ILE:CD1	23:Q:92:ARG:HB2	2.50	0.41
27:U:86:ARG:NH1	27:U:100:SER:OG	2.52	0.41
36:d:18:PHE:HA	36:d:43:THR:HG21	2.03	0.41
47:o:22:THR:HA	47:o:25:ILE:HG22	2.02	0.41
49:q:81:LEU:HD22	49:q:101:ALA:HB1	2.01	0.41
51:s:49:GLN:OE1	56:x:12:ASP:HA	2.20	0.41
1:1:26:G:C6	1:1:27:G:N1	2.88	0.41
1:1:735:A:C8	1:1:736:C:C5	3.08	0.41
1:1:2222:C:H2'	1:1:2223:G:O4'	2.20	0.41
1:1:2298:A:C5	1:1:2321:U:C4	3.08	0.41
2:2:567:G:H2'	2:2:568:G:O5'	2.20	0.41
14:H:18:VAL:HG22	14:H:86:MET:HE2	2.01	0.41
15:I:37:PHE:CE1	15:I:58:ILE:HG23	2.55	0.41
32:Z:7:ILE:CD1	32:Z:27:LEU:HD22	2.50	0.41
36:d:31:LEU:HD22	36:d:42:LEU:CD1	2.50	0.41
51:s:42:TRP:HA	51:s:45:VAL:HG13	2.02	0.41
1:1:875:G:C6	1:1:876:C:C4	3.08	0.41
1:1:1525:A:C5	1:1:1526:C:C5	3.09	0.41
2:2:1007:U:N3	2:2:1022:A:N1	2.67	0.41
32:Z:25:LEU:C	32:Z:25:LEU:HD13	2.45	0.41
36:d:5:PHE:CE2	36:d:7:PRO:HB3	2.55	0.41
40:h:120:ILE:HD11	40:h:137:ALA:CB	2.49	0.41
41:i:37:ALA:HB1	41:i:38:PRO:HD2	2.02	0.41
1:1:679:C:H2'	1:1:680:C:H6	1.85	0.41
1:1:930:G:H1'	32:Z:25:LEU:HD11	2.03	0.41
1:1:2602:A:H5''	1:1:2603:G:C5'	2.50	0.41
2:2:563:A:N6	2:2:567:G:C2	2.88	0.41
2:2:723:U:C6	58:z:52:ALA:HB1	2.55	0.41
2:2:1060:U:OP1	51:s:85:ARG:NH1	2.54	0.41
2:2:1439:G:H2'	2:2:1440:U:O4'	2.21	0.41
24:R:3:ALA:HB3	24:R:59:ILE:HD11	2.02	0.41
29:W:52:GLY:O	29:W:59:LEU:HA	2.19	0.41
1:1:591:U:O2	37:e:2:PRO:N	2.54	0.41
1:1:1357:C:H2'	1:1:1358:G:O4'	2.20	0.41
1:1:1779:U:C2	1:1:1783:A:N7	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:553:A:H5''	49:q:21:VAL:HG21	2.03	0.41
11:E:122:PHE:CZ	11:E:167:ARG:HA	2.56	0.41
21:O:27:VAL:CG2	21:O:40:ILE:HD12	2.51	0.41
1:1:565:C:H2'	1:1:566:U:O4'	2.20	0.41
1:1:1172:C:H2'	1:1:1173:U:O4'	2.21	0.41
2:2:622:A:C8	2:2:623:C:C5	3.08	0.41
8:B:34:LEU:HA	8:B:62:TYR:O	2.21	0.41
14:H:53:ARG:HB2	14:H:55:VAL:HG13	2.01	0.41
15:I:12:VAL:HG21	15:I:22:PRO:HG3	2.02	0.41
23:Q:76:TYR:CZ	23:Q:80:ILE:HG13	2.55	0.41
33:a:41:HIS:CD2	33:a:42:PRO:HD2	2.56	0.41
39:g:114:LEU:HD13	39:g:144:LEU:HB3	2.03	0.41
47:o:11:LYS:HA	47:o:18:ILE:HD11	2.02	0.41
49:q:3:THR:O	49:q:6:GLN:HB2	2.21	0.41
51:s:80:SER:O	51:s:84:VAL:HG23	2.21	0.41
2:2:108:G:N3	2:2:108:G:O4'	2.53	0.41
2:2:429:U:H3'	41:i:9:LEU:HD12	2.02	0.41
2:2:1279:G:O2'	2:2:1281:C:OP2	2.28	0.41
3:3:8:C:O3'	21:O:25:ARG:NH1	2.53	0.41
12:F:26:ILE:HG22	12:F:79:VAL:HG21	2.02	0.41
15:I:109:ALA:HB2	15:I:128:ILE:CD1	2.49	0.41
41:i:91:LEU:HD23	41:i:91:LEU:HA	1.87	0.41
42:j:114:VAL:HG21	42:j:141:ILE:HD12	2.03	0.41
43:k:27:ALA:O	43:k:30:THR:OG1	2.29	0.41
47:o:53:ILE:HG22	51:s:85:ARG:HD2	2.03	0.41
1:1:12:U:O2	1:1:12:U:H2'	2.21	0.41
1:1:479:A:H4'	1:1:480:A:OP1	2.21	0.41
1:1:910:A:N1	1:1:2277:G:H1'	2.36	0.41
1:1:1401:G:C5	1:1:1402:U:C4	3.09	0.41
1:1:1406:U:O2'	1:1:1407:G:C5'	2.69	0.41
1:1:2096:C:H2'	1:1:2097:A:O4'	2.21	0.41
1:1:2233:U:H2'	1:1:2234:G:C8	2.55	0.41
1:1:2297:A:C6	1:1:2321:U:O4	2.73	0.41
2:2:66:A:C6	2:2:67:C:C5	3.09	0.41
2:2:694:A:N1	2:2:787:A:O2'	2.54	0.41
2:2:1181:G:O2'	2:2:1182:G:N7	2.50	0.41
2:2:1497:G:H2'	2:2:1498:UR3:H6	2.02	0.41
7:7:197:ALA:HB2	7:7:223:VAL:HG23	2.01	0.41
7:7:332:ASN:HA	7:7:346:PRO:HG2	2.02	0.41
8:B:154:LEU:HD13	8:B:176:LEU:HD21	2.02	0.41
8:B:240:PHE:O	8:B:240:PHE:CG	2.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:57:LYS:O	13:G:61:VAL:HG13	2.21	0.41
16:J:92:MET:HE1	16:J:103:ILE:HD12	2.03	0.41
18:L:82:LEU:O	18:L:85:VAL:HG22	2.21	0.41
42:j:56:VAL:HB	42:j:57:PRO:HD3	2.02	0.41
48:p:19:GLY:O	48:p:82:LEU:HD12	2.21	0.41
49:q:42:PRO:HA	49:q:90:LEU:HD23	2.03	0.41
54:v:17:MET:HE1	54:v:45:HIS:ND1	2.36	0.41
58:z:42:THR:OG1	58:z:43:THR:N	2.54	0.41
2:2:6:G:C4	42:j:124:LEU:HD11	2.56	0.41
2:2:198:G:H2'	2:2:199:A:C8	2.55	0.41
3:3:89:U:O2	3:3:89:U:O4'	2.37	0.41
5:5:44:A:H2'	5:5:45:G:O4'	2.21	0.41
7:7:155:ARG:CB	7:7:351:ASP:O	2.69	0.41
10:D:148:ILE:O	10:D:169:VAL:HA	2.21	0.41
20:N:12:ARG:O	20:N:17:ARG:NH2	2.53	0.41
28:V:15:GLY:O	28:V:19:ARG:HG3	2.21	0.41
40:h:153:VAL:HG12	40:h:198:VAL:HG13	2.02	0.41
1:1:152:A:H2'	1:1:153:U:O4'	2.21	0.40
2:2:1225:A:N3	2:2:1225:A:C2'	2.84	0.40
2:2:1523:G:OP1	48:p:125:LYS:HD2	2.21	0.40
8:B:51:THR:CG2	8:B:54:ILE:HD12	2.50	0.40
19:M:46:ILE:HD12	19:M:69:PRO:HG3	2.04	0.40
24:R:74:ILE:N	24:R:74:ILE:HD12	2.36	0.40
40:h:114:LYS:HA	40:h:185:ASN:HB3	2.03	0.40
42:j:154:ALA:O	42:j:158:GLY:N	2.54	0.40
45:m:7:ILE:HD11	45:m:32:LEU:HD23	2.02	0.40
47:o:52:LEU:HD13	47:o:58:ASN:O	2.20	0.40
1:1:88:G:C6	1:1:89:A:N7	2.89	0.40
1:1:160:A:C6	1:1:161:A:C6	3.09	0.40
1:1:340:A:O2'	10:D:162:ARG:NH1	2.54	0.40
1:1:888:C:C5	50:r:92:ARG:HD2	2.56	0.40
2:2:915:A:C6	2:2:916:U:C4	3.08	0.40
8:B:76:ALA:HB2	8:B:96:TYR:CE1	2.56	0.40
10:D:48:THR:HG23	10:D:86:ALA:HB3	2.02	0.40
16:J:73:VAL:HG11	16:J:75:TYR:CZ	2.56	0.40
1:1:928:A:H2'	1:1:929:U:O4'	2.22	0.40
1:1:2314:A:H2'	1:1:2315:G:C8	2.56	0.40
2:2:664:G:H22	2:2:741:G:H1	1.67	0.40
2:2:946:A:C2	2:2:1236:A:C2	3.09	0.40
2:2:960:U:O2'	2:2:1223:C:H4'	2.21	0.40
8:B:157:SER:O	8:B:195:VAL:HG11	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:20:SER:N	15:I:21:PRO:CD	2.84	0.40
23:Q:82:GLY:HA2	23:Q:117:LEU:HD12	2.04	0.40
27:U:94:ARG:CB	27:U:103:ILE:HD12	2.49	0.40
38:f:33:HIS:O	38:f:35:GLN:NE2	2.55	0.40
48:p:34:ILE:HG12	48:p:70:CYS:SG	2.61	0.40
1:1:36:G:N3	1:1:450:G:O2'	2.53	0.40
1:1:126:A:OP2	36:d:19:ARG:HG3	2.22	0.40
1:1:493:G:H2'	1:1:494:G:O4'	2.20	0.40
1:1:861:A:H2'	1:1:862:G:O4'	2.21	0.40
1:1:2850:A:N7	1:1:2868:A:O2'	2.36	0.40
2:2:140:U:H2'	2:2:141:G:O4'	2.21	0.40
2:2:685:G:N1	2:2:686:U:O4	2.55	0.40
2:2:1345:U:C2	2:2:1377:A:C2	3.10	0.40
7:7:44:ARG:O	7:7:44:ARG:HD2	2.21	0.40
12:F:52:PHE:CD2	12:F:69:ARG:HB2	2.57	0.40
23:Q:61:TRP:CH2	23:Q:93:LYS:HB2	2.56	0.40
42:j:46:VAL:HG12	42:j:47:GLY:N	2.36	0.40
1:1:1107:G:O2'	14:H:81:LEU:HD23	2.22	0.40
1:1:1153:C:H2'	1:1:1154:G:O4'	2.21	0.40
2:2:181:A:O2'	2:2:194:C:N4	2.54	0.40
2:2:915:A:N6	2:2:916:U:O4	2.53	0.40
7:7:42:LEU:HD23	7:7:68:LEU:CD2	2.51	0.40
7:7:201:ARG:HB2	7:7:323:GLN:HG2	2.03	0.40
8:B:76:ALA:HB2	8:B:96:TYR:CD1	2.56	0.40
47:o:17:LEU:HD22	47:o:96:VAL:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	6	30/61 (49%)	27 (90%)	3 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	7	316/378 (84%)	287 (91%)	26 (8%)	3 (1%)	14	41
8	B	269/273 (98%)	252 (94%)	15 (6%)	2 (1%)	18	46
9	C	207/209 (99%)	191 (92%)	15 (7%)	1 (0%)	24	52
10	D	199/201 (99%)	191 (96%)	7 (4%)	1 (0%)	24	52
11	E	175/179 (98%)	160 (91%)	12 (7%)	3 (2%)	7	27
12	F	173/177 (98%)	162 (94%)	11 (6%)	0	100	100
13	G	144/149 (97%)	133 (92%)	10 (7%)	1 (1%)	18	46
14	H	128/165 (78%)	107 (84%)	18 (14%)	3 (2%)	5	22
15	I	133/142 (94%)	116 (87%)	16 (12%)	1 (1%)	16	44
16	J	140/142 (99%)	132 (94%)	7 (5%)	1 (1%)	18	46
17	K	121/123 (98%)	111 (92%)	10 (8%)	0	100	100
18	L	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
19	M	134/136 (98%)	126 (94%)	8 (6%)	0	100	100
20	N	117/127 (92%)	112 (96%)	5 (4%)	0	100	100
21	O	114/117 (97%)	106 (93%)	7 (6%)	1 (1%)	14	41
22	P	112/115 (97%)	106 (95%)	6 (5%)	0	100	100
23	Q	115/118 (98%)	110 (96%)	3 (3%)	2 (2%)	7	27
24	R	101/103 (98%)	91 (90%)	10 (10%)	0	100	100
25	S	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
26	T	92/100 (92%)	88 (96%)	4 (4%)	0	100	100
27	U	101/104 (97%)	91 (90%)	9 (9%)	1 (1%)	12	38
28	V	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
29	W	74/85 (87%)	69 (93%)	5 (7%)	0	100	100
30	X	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
31	Y	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
32	Z	56/59 (95%)	53 (95%)	2 (4%)	1 (2%)	6	26
33	a	61/70 (87%)	56 (92%)	5 (8%)	0	100	100
34	b	54/57 (95%)	49 (91%)	5 (9%)	0	100	100
35	c	50/55 (91%)	44 (88%)	6 (12%)	0	100	100
36	d	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
37	e	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	3	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	f	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
39	g	223/241 (92%)	207 (93%)	15 (7%)	1 (0%)	30	58
40	h	206/233 (88%)	191 (93%)	14 (7%)	1 (0%)	24	52
41	i	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
42	j	154/167 (92%)	148 (96%)	5 (3%)	1 (1%)	21	49
43	k	102/135 (76%)	94 (92%)	7 (7%)	1 (1%)	12	38
44	l	149/179 (83%)	143 (96%)	3 (2%)	3 (2%)	6	24
45	m	127/130 (98%)	120 (94%)	6 (5%)	1 (1%)	16	44
46	n	125/130 (96%)	117 (94%)	7 (6%)	1 (1%)	16	44
47	o	97/103 (94%)	92 (95%)	5 (5%)	0	100	100
48	p	115/129 (89%)	100 (87%)	14 (12%)	1 (1%)	14	41
49	q	120/124 (97%)	115 (96%)	5 (4%)	0	100	100
50	r	114/118 (97%)	106 (93%)	7 (6%)	1 (1%)	14	41
51	s	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
52	t	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
53	u	80/82 (98%)	73 (91%)	7 (9%)	0	100	100
54	v	78/84 (93%)	70 (90%)	8 (10%)	0	100	100
55	w	64/75 (85%)	62 (97%)	2 (3%)	0	100	100
56	x	81/92 (88%)	79 (98%)	2 (2%)	0	100	100
57	y	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
58	z	68/71 (96%)	68 (100%)	0	0	100	100
All	All	6209/6659 (93%)	5804 (94%)	371 (6%)	34 (0%)	26	52

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	7	128	ASN
9	C	150	GLN
14	H	117	LEU
46	n	56	ASP
7	7	93	PRO
8	B	241	GLY
11	E	177	PHE
21	O	100	HIS
23	Q	3	ARG

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Mol	Chain	Res	Type
37	e	28	ASN
7	7	197	ALA
8	B	158	ALA
10	D	142	ALA
16	J	100	VAL
32	Z	3	LYS
27	U	99	ASN
40	h	17	PRO
42	j	44	GLY
43	k	96	VAL
44	l	130	ASN
44	l	150	ALA
50	r	66	GLU
11	E	42	GLU
14	H	109	LYS
11	E	40	VAL
13	G	10	ALA
14	H	51	TYR
37	e	32	ILE
45	m	75	ILE
15	I	136	GLY
23	Q	74	ILE
39	g	98	GLY
48	p	74	VAL
44	l	71	PRO

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	
6	6	26/51 (51%)	20 (77%)	6 (23%)	1	2
7	7	275/319 (86%)	221 (80%)	54 (20%)	1	5
8	B	216/218 (99%)	196 (91%)	20 (9%)	8	30
9	C	164/164 (100%)	157 (96%)	7 (4%)	26	52
10	D	165/165 (100%)	151 (92%)	14 (8%)	10	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	E	148/150 (99%)	132 (89%)	16 (11%)	6	22
12	F	136/138 (99%)	123 (90%)	13 (10%)	8	29
13	G	112/114 (98%)	93 (83%)	19 (17%)	2	9
14	H	99/123 (80%)	85 (86%)	14 (14%)	3	13
15	I	104/110 (94%)	97 (93%)	7 (7%)	15	41
16	J	116/116 (100%)	105 (90%)	11 (10%)	8	29
17	K	104/104 (100%)	94 (90%)	10 (10%)	8	29
18	L	103/103 (100%)	94 (91%)	9 (9%)	9	32
19	M	109/109 (100%)	97 (89%)	12 (11%)	6	22
20	N	99/103 (96%)	88 (89%)	11 (11%)	6	21
21	O	86/87 (99%)	79 (92%)	7 (8%)	11	36
22	P	99/100 (99%)	87 (88%)	12 (12%)	5	18
23	Q	89/90 (99%)	81 (91%)	8 (9%)	9	31
24	R	84/84 (100%)	77 (92%)	7 (8%)	10	35
25	S	93/93 (100%)	85 (91%)	8 (9%)	10	33
26	T	81/84 (96%)	72 (89%)	9 (11%)	6	21
27	U	84/85 (99%)	76 (90%)	8 (10%)	8	29
28	V	78/78 (100%)	71 (91%)	7 (9%)	9	31
29	W	58/63 (92%)	56 (97%)	2 (3%)	32	58
30	X	67/68 (98%)	63 (94%)	4 (6%)	17	44
31	Y	54/55 (98%)	49 (91%)	5 (9%)	8	30
32	Z	48/49 (98%)	37 (77%)	11 (23%)	1	2
33	a	56/62 (90%)	49 (88%)	7 (12%)	4	17
34	b	47/48 (98%)	39 (83%)	8 (17%)	2	9
35	c	47/49 (96%)	42 (89%)	5 (11%)	6	23
36	d	38/38 (100%)	33 (87%)	5 (13%)	4	15
37	e	51/52 (98%)	48 (94%)	3 (6%)	18	44
38	f	34/34 (100%)	29 (85%)	5 (15%)	3	12
39	g	187/199 (94%)	177 (95%)	10 (5%)	20	48
40	h	171/190 (90%)	158 (92%)	13 (8%)	12	38
41	i	172/173 (99%)	166 (96%)	6 (4%)	32	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	j	119/126 (94%)	104 (87%)	15 (13%)	4	17
43	k	91/116 (78%)	83 (91%)	8 (9%)	9	31
44	l	124/147 (84%)	106 (86%)	18 (14%)	3	13
45	m	104/105 (99%)	98 (94%)	6 (6%)	18	45
46	n	105/107 (98%)	94 (90%)	11 (10%)	6	24
47	o	86/90 (96%)	76 (88%)	10 (12%)	5	20
48	p	90/99 (91%)	85 (94%)	5 (6%)	19	46
49	q	102/103 (99%)	91 (89%)	11 (11%)	6	22
50	r	94/96 (98%)	86 (92%)	8 (8%)	10	33
51	s	83/84 (99%)	80 (96%)	3 (4%)	31	56
52	t	76/77 (99%)	66 (87%)	10 (13%)	4	15
53	u	65/65 (100%)	59 (91%)	6 (9%)	8	30
54	v	74/78 (95%)	69 (93%)	5 (7%)	14	41
55	w	57/65 (88%)	52 (91%)	5 (9%)	9	31
56	x	72/79 (91%)	67 (93%)	5 (7%)	14	40
57	y	65/66 (98%)	63 (97%)	2 (3%)	35	59
58	z	60/61 (98%)	52 (87%)	8 (13%)	4	15
All	All	5167/5432 (95%)	4658 (90%)	509 (10%)	10	27

All (509) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	6	16	ILE
6	6	17	GLU
6	6	19	LEU
6	6	20	LEU
6	6	24	LEU
6	6	36	LYS
7	7	20	ARG
7	7	29	ILE
7	7	31	ASP
7	7	35	LYS
7	7	38	ARG
7	7	42	LEU
7	7	45	ARG
7	7	46	LEU

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Mol	Chain	Res	Type
7	7	52	TRP
7	7	59	ARG
7	7	63	GLN
7	7	68	LEU
7	7	74	THR
7	7	81	ASP
7	7	88	LEU
7	7	98	GLU
7	7	101	LYS
7	7	105	GLU
7	7	111	LEU
7	7	119	LEU
7	7	121	ASN
7	7	128	ASN
7	7	131	LEU
7	7	145	TRP
7	7	149	LEU
7	7	151	ARG
7	7	152	MET
7	7	158	GLU
7	7	160	GLN
7	7	174	GLU
7	7	177	ILE
7	7	182	ILE
7	7	183	LEU
7	7	185	LYS
7	7	188	ASN
7	7	192	LEU
7	7	196	GLU
7	7	222	GLU
7	7	227	VAL
7	7	236	LYS
7	7	240	LEU
7	7	274	THR
7	7	279	ARG
7	7	290	LYS
7	7	296	LEU
7	7	322	SER
7	7	323	GLN
7	7	324	ILE
7	7	325	ARG
7	7	331	LYS

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Mol	Chain	Res	Type
7	7	333	TYR
7	7	338	ARG
7	7	358	ILE
7	7	368	ARG
8	B	13	ARG
8	B	35	GLU
8	B	40	SER
8	B	94	VAL
8	B	125	LYS
8	B	130	LEU
8	B	141	VAL
8	B	153	GLN
8	B	156	ARG
8	B	174	LEU
8	B	180	GLU
8	B	181	MET
8	B	192	LEU
8	B	203	ARG
8	B	204	VAL
8	B	205	LEU
8	B	242	LYS
8	B	244	PRO
8	B	257	THR
8	B	271	ARG
9	C	2	ILE
9	C	13	ARG
9	C	46	ARG
9	C	50	VAL
9	C	149	ASN
9	C	177	VAL
9	C	207	VAL
10	D	15	SER
10	D	16	GLU
10	D	57	LYS
10	D	69	ARG
10	D	73	ILE
10	D	77	ILE
10	D	96	VAL
10	D	108	ILE
10	D	109	LEU
10	D	122	GLU
10	D	149	ILE

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Mol	Chain	Res	Type
10	D	152	GLU
10	D	163	ASN
10	D	195	GLN
11	E	9	LYS
11	E	10	ASP
11	E	26	MET
11	E	40	VAL
11	E	47	LYS
11	E	49	LEU
11	E	57	LEU
11	E	95	ARG
11	E	112	ARG
11	E	117	LEU
11	E	123	ASP
11	E	132	VAL
11	E	140	GLU
11	E	141	ILE
11	E	163	ASP
11	E	175	PHE
12	F	6	LYS
12	F	11	VAL
12	F	20	ASN
12	F	39	ASP
12	F	50	LEU
12	F	72	LEU
12	F	76	VAL
12	F	89	LEU
12	F	95	ARG
12	F	117	LEU
12	F	133	LEU
12	F	141	ILE
12	F	152	ARG
13	G	4	ILE
13	G	15	LEU
13	G	18	GLN
13	G	20	ASN
13	G	33	GLN
13	G	35	LYS
13	G	40	THR
13	G	41	LYS
13	G	43	ASN
13	G	44	ILE

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Mol	Chain	Res	Type
13	G	50	ARG
13	G	51	ARG
13	G	66	ASN
13	G	72	ILE
13	G	77	THR
13	G	87	GLU
13	G	94	ILE
13	G	101	ASP
13	G	114	GLU
14	H	3	LEU
14	H	34	THR
14	H	37	LYS
14	H	38	MET
14	H	40	GLU
14	H	54	VAL
14	H	57	ASN
14	H	65	GLU
14	H	70	GLU
14	H	107	GLU
14	H	108	VAL
14	H	109	LYS
14	H	122	GLN
14	H	123	ILE
15	I	10	LEU
15	I	11	GLN
15	I	38	CYS
15	I	42	ASN
15	I	63	ASP
15	I	78	LEU
15	I	85	ILE
16	J	12	LYS
16	J	19	ASP
16	J	30	THR
16	J	40	HIS
16	J	43	GLU
16	J	81	ILE
16	J	124	VAL
16	J	128	ASN
16	J	129	GLU
16	J	140	LEU
16	J	142	ILE
17	K	7	MET

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Mol	Chain	Res	Type
17	K	8	LEU
17	K	58	LEU
17	K	67	LYS
17	K	70	ARG
17	K	80	ASP
17	K	97	THR
17	K	104	THR
17	K	105	ARG
17	K	111	LYS
18	L	4	ASN
18	L	18	ARG
18	L	23	ILE
18	L	39	LYS
18	L	46	VAL
18	L	59	ARG
18	L	78	ARG
18	L	84	LYS
18	L	86	GLU
19	M	2	LEU
19	M	3	GLN
19	M	47	GLU
19	M	63	ILE
19	M	80	VAL
19	M	84	LYS
19	M	100	LYS
19	M	110	GLU
19	M	119	LEU
19	M	126	ILE
19	M	132	THR
19	M	133	LYS
20	N	17	ARG
20	N	20	MET
20	N	43	GLU
20	N	51	LEU
20	N	52	ILE
20	N	59	SER
20	N	63	ARG
20	N	65	LEU
20	N	69	ARG
20	N	76	VAL
20	N	79	LEU
21	O	19	GLN

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Mol	Chain	Res	Type
21	O	31	THR
21	O	48	LEU
21	O	67	ASN
21	O	87	ILE
21	O	98	GLN
21	O	116	GLN
22	P	10	GLN
22	P	11	GLU
22	P	21	ARG
22	P	26	VAL
22	P	38	LYS
22	P	81	VAL
22	P	89	ARG
22	P	92	VAL
22	P	102	GLU
22	P	110	ILE
22	P	111	LYS
22	P	113	ARG
23	Q	11	ARG
23	Q	17	ILE
23	Q	18	LEU
23	Q	22	LYS
23	Q	51	ARG
23	Q	71	GLN
23	Q	87	SER
23	Q	91	ASP
24	R	4	VAL
24	R	6	GLN
24	R	10	LYS
24	R	14	VAL
24	R	39	LEU
24	R	86	GLN
24	R	95	ASP
25	S	4	ILE
25	S	11	ARG
25	S	19	LEU
25	S	41	LYS
25	S	50	VAL
25	S	69	LEU
25	S	81	SER
25	S	105	VAL
26	T	2	ILE

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Mol	Chain	Res	Type
26	T	6	ARG
26	T	11	LEU
26	T	16	VAL
26	T	25	GLU
26	T	33	LYS
26	T	78	SER
26	T	87	LEU
26	T	93	LEU
27	U	7	ARG
27	U	10	GLU
27	U	15	THR
27	U	52	LEU
27	U	62	GLU
27	U	68	SER
27	U	81	ASP
27	U	88	GLU
28	V	1	MET
28	V	5	ASN
28	V	20	LEU
28	V	29	ILE
28	V	34	LYS
28	V	40	ILE
28	V	69	GLU
29	W	10	THR
29	W	77	ARG
30	X	35	SER
30	X	48	THR
30	X	56	MET
30	X	76	GLU
31	Y	7	ARG
31	Y	18	LEU
31	Y	57	LEU
31	Y	58	ASN
31	Y	60	LYS
32	Z	5	ILE
32	Z	10	THR
32	Z	11	ARG
32	Z	14	ILE
32	Z	24	LEU
32	Z	25	LEU
32	Z	36	VAL
32	Z	41	THR

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Mol	Chain	Res	Type
32	Z	45	ARG
32	Z	49	ASN
32	Z	57	VAL
33	a	5	ILE
33	a	8	LYS
33	a	18	CYS
33	a	24	ILE
33	a	37	CYS
33	a	45	THR
33	a	59	ARG
34	b	8	PRO
34	b	9	THR
34	b	11	SER
34	b	26	THR
34	b	36	GLU
34	b	40	ARG
34	b	52	ARG
34	b	55	ILE
35	c	34	LEU
35	c	43	VAL
35	c	47	VAL
35	c	53	LYS
35	c	55	LYS
36	d	22	MET
36	d	24	THR
36	d	31	LEU
36	d	42	LEU
36	d	44	VAL
37	e	3	LYS
37	e	30	ARG
37	e	55	LEU
38	f	3	VAL
38	f	7	VAL
38	f	11	CYS
38	f	26	ILE
38	f	27	CYS
39	g	4	VAL
39	g	5	SER
39	g	59	LYS
39	g	105	LYS
39	g	128	LYS
39	g	129	LEU

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Mol	Chain	Res	Type
39	g	135	LEU
39	g	161	LEU
39	g	212	LEU
39	g	227	GLN
40	h	14	ILE
40	h	16	LYS
40	h	89	LYS
40	h	97	VAL
40	h	149	ILE
40	h	151	VAL
40	h	154	SER
40	h	165	THR
40	h	172	ARG
40	h	175	LEU
40	h	178	LEU
40	h	179	ARG
40	h	200	VAL
41	i	5	LEU
41	i	95	GLU
41	i	104	ARG
41	i	116	GLN
41	i	138	SER
41	i	143	VAL
42	j	15	LEU
42	j	34	THR
42	j	60	ILE
42	j	65	GLU
42	j	72	ILE
42	j	94	VAL
42	j	114	VAL
42	j	115	LEU
42	j	120	VAL
42	j	123	VAL
42	j	126	LYS
42	j	138	ARG
42	j	141	ILE
42	j	149	SER
42	j	165	LEU
43	k	7	VAL
43	k	16	GLU
43	k	24	ARG
43	k	38	ARG

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Mol	Chain	Res	Type
43	k	54	LEU
43	k	71	ILE
43	k	86	ARG
43	k	103	VAL
44	l	7	ILE
44	l	11	LYS
44	l	17	LYS
44	l	21	GLU
44	l	23	LEU
44	l	27	VAL
44	l	40	GLU
44	l	47	LEU
44	l	50	LEU
44	l	79	ARG
44	l	87	VAL
44	l	91	VAL
44	l	109	ARG
44	l	123	GLU
44	l	126	ASP
44	l	142	HIS
44	l	144	MET
44	l	146	GLU
45	m	9	ASP
45	m	12	THR
45	m	77	ARG
45	m	96	MET
45	m	104	VAL
45	m	107	SER
46	n	25	ASN
46	n	27	LYS
46	n	60	LYS
46	n	61	LEU
46	n	63	LEU
46	n	85	ARG
46	n	98	LEU
46	n	116	VAL
46	n	118	LEU
46	n	123	ARG
46	n	130	ARG
47	o	17	LEU
47	o	18	ILE
47	o	24	GLU

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Mol	Chain	Res	Type
47	o	25	ILE
47	o	27	GLU
47	o	37	ARG
47	o	57	VAL
47	o	63	ASP
47	o	90	LEU
47	o	92	LEU
48	p	13	ARG
48	p	15	GLN
48	p	18	ASP
48	p	100	LEU
48	p	107	ILE
49	q	12	ARG
49	q	21	VAL
49	q	24	LEU
49	q	30	LYS
49	q	62	GLU
49	q	64	THR
49	q	74	LEU
49	q	81	LEU
49	q	86	ARG
49	q	87	VAL
49	q	102	LEU
50	r	9	ILE
50	r	16	VAL
50	r	25	VAL
50	r	29	ARG
50	r	59	GLU
50	r	68	ASP
50	r	89	LEU
50	r	93	ARG
51	s	7	LYS
51	s	45	VAL
51	s	92	GLU
52	t	22	THR
52	t	39	LEU
52	t	40	GLN
52	t	64	ARG
52	t	66	LEU
52	t	67	LEU
52	t	73	LYS
52	t	80	GLN

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Mol	Chain	Res	Type
52	t	84	ARG
52	t	85	LEU
53	u	2	VAL
53	u	3	THR
53	u	18	GLN
53	u	19	VAL
53	u	20	VAL
53	u	76	LYS
54	v	22	VAL
54	v	67	LEU
54	v	74	THR
54	v	75	LEU
54	v	81	LYS
55	w	12	ARG
55	w	14	THR
55	w	66	SER
55	w	71	THR
55	w	74	HIS
56	x	21	LYS
56	x	33	THR
56	x	49	ILE
56	x	58	VAL
56	x	81	ARG
57	y	48	GLN
57	y	57	ILE
58	z	4	ILE
58	z	28	VAL
58	z	31	GLU
58	z	55	ARG
58	z	59	LYS
58	z	62	ARG
58	z	67	ARG
58	z	70	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
7	7	134	GLN
7	7	188	ASN
7	7	332	ASN
8	B	25	HIS
8	B	37	ASN

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Mol	Chain	Res	Type
8	B	117	GLN
8	B	163	GLN
9	C	94	GLN
9	C	140	HIS
9	C	149	ASN
10	D	46	GLN
11	E	5	HIS
12	F	20	ASN
12	F	116	GLN
13	G	2	GLN
13	G	20	ASN
13	G	145	ASN
15	I	30	GLN
15	I	93	ASN
16	J	130	HIS
18	L	4	ASN
20	N	73	ASN
21	O	38	GLN
22	P	7	GLN
22	P	41	GLN
22	P	56	HIS
22	P	66	ASN
22	P	115	ASN
23	Q	14	HIS
23	Q	72	ASN
24	R	18	GLN
27	U	54	GLN
28	V	5	ASN
31	Y	58	ASN
33	a	61	ASN
39	g	19	GLN
39	g	58	ASN
39	g	89	GLN
40	h	6	HIS
40	h	123	GLN
41	i	126	ASN
42	j	97	GLN
43	k	11	HIS
48	p	15	GLN
48	p	38	GLN
52	t	35	GLN
52	t	80	GLN

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Mol	Chain	Res	Type
53	u	18	GLN
57	y	3	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2902/2904 (99%)	631 (21%)	91 (3%)
2	2	1531/1534 (99%)	336 (21%)	39 (2%)
3	3	119/120 (99%)	20 (16%)	1 (0%)
4	4	4/18 (22%)	1 (25%)	0
5	5	74/78 (94%)	24 (32%)	7 (9%)
All	All	4630/4654 (99%)	1012 (21%)	138 (2%)

All (1012) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	A
1	1	15	G
1	1	23	G
1	1	34	U
1	1	35	G
1	1	45	G
1	1	46	G
1	1	58	G
1	1	60	G
1	1	62	U
1	1	63	A
1	1	71	A
1	1	72	U
1	1	74	A
1	1	75	G
1	1	80	G
1	1	83	A
1	1	84	A
1	1	85	G
1	1	101	A
1	1	102	U
1	1	103	A
1	1	118	A
1	1	119	A
1	1	120	U

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Mol	Chain	Res	Type
1	1	131	A
1	1	137	U
1	1	138	U
1	1	139	U
1	1	140	C
1	1	141	G
1	1	142	A
1	1	143	C
1	1	144	A
1	1	149	A
1	1	163	C
1	1	165	A
1	1	181	A
1	1	186	G
1	1	196	A
1	1	197	A
1	1	199	A
1	1	200	U
1	1	215	G
1	1	216	A
1	1	222	A
1	1	225	C
1	1	241	A
1	1	248	G
1	1	249	C
1	1	264	C
1	1	265	A
1	1	266	G
1	1	271	G
1	1	272	A
1	1	275	C
1	1	276	U
1	1	278	A
1	1	279	A
1	1	285	G
1	1	291	G
1	1	303	G
1	1	311	A
1	1	312	G
1	1	324	A
1	1	327	G
1	1	329	G

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Mol	Chain	Res	Type
1	1	330	A
1	1	353	C
1	1	361	G
1	1	362	A
1	1	366	C
1	1	371	A
1	1	372	G
1	1	386	G
1	1	396	G
1	1	405	U
1	1	406	G
1	1	411	G
1	1	412	A
1	1	416	U
1	1	417	C
1	1	420	C
1	1	424	G
1	1	450	G
1	1	451	U
1	1	455	C
1	1	457	A
1	1	459	U
1	1	467	G
1	1	477	A
1	1	480	A
1	1	481	G
1	1	490	C
1	1	491	G
1	1	501	A
1	1	503	A
1	1	504	A
1	1	505	A
1	1	509	C
1	1	519	U
1	1	522	A
1	1	530	G
1	1	531	C
1	1	532	A
1	1	533	G
1	1	543	G
1	1	546	U
1	1	547	A

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Mol	Chain	Res	Type
1	1	548	G
1	1	549	G
1	1	551	G
1	1	563	A
1	1	572	A
1	1	573	U
1	1	575	A
1	1	586	A
1	1	603	A
1	1	609	A
1	1	613	A
1	1	614	A
1	1	615	U
1	1	616	A
1	1	618	G
1	1	620	G
1	1	621	A
1	1	627	A
1	1	637	A
1	1	645	C
1	1	647	G
1	1	654	A
1	1	659	G
1	1	664	G
1	1	668	A
1	1	670	A
1	1	682	G
1	1	683	U
1	1	685	A
1	1	686	U
1	1	701	G
1	1	709	U
1	1	710	U
1	1	716	A
1	1	717	C
1	1	724	U
1	1	730	A
1	1	735	A
1	1	738	G
1	1	745	1MG
1	1	746	PSU
1	1	747	5MU

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Mol	Chain	Res	Type
1	1	757	G
1	1	764	A
1	1	765	C
1	1	775	G
1	1	776	G
1	1	782	A
1	1	784	G
1	1	785	G
1	1	786	C
1	1	805	G
1	1	812	C
1	1	819	A
1	1	827	U
1	1	828	U
1	1	831	G
1	1	845	A
1	1	846	U
1	1	858	G
1	1	859	G
1	1	878	A
1	1	881	G
1	1	883	G
1	1	884	U
1	1	885	C
1	1	887	A
1	1	888	C
1	1	891	G
1	1	892	A
1	1	893	C
1	1	895	U
1	1	896	A
1	1	897	C
1	1	899	A
1	1	907	G
1	1	910	A
1	1	914	G
1	1	931	U
1	1	941	A
1	1	945	A
1	1	946	C
1	1	953	G
1	1	961	C

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Mol	Chain	Res	Type
1	1	974	G
1	1	983	A
1	1	989	G
1	1	995	C
1	1	996	A
1	1	999	U
1	1	1005	C
1	1	1012	U
1	1	1013	C
1	1	1022	G
1	1	1023	U
1	1	1026	G
1	1	1033	U
1	1	1041	G
1	1	1043	C
1	1	1045	C
1	1	1046	A
1	1	1047	G
1	1	1060	U
1	1	1061	U
1	1	1062	G
1	1	1063	G
1	1	1064	C
1	1	1065	U
1	1	1066	U
1	1	1067	A
1	1	1068	G
1	1	1070	A
1	1	1073	A
1	1	1074	G
1	1	1076	C
1	1	1079	C
1	1	1080	A
1	1	1081	U
1	1	1082	U
1	1	1083	U
1	1	1084	A
1	1	1087	G
1	1	1088	A
1	1	1090	A
1	1	1094	U
1	1	1095	A

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Mol	Chain	Res	Type
1	1	1096	A
1	1	1097	U
1	1	1109	C
1	1	1110	G
1	1	1111	A
1	1	1112	G
1	1	1119	U
1	1	1128	G
1	1	1129	A
1	1	1130	U
1	1	1132	U
1	1	1133	A
1	1	1134	A
1	1	1135	C
1	1	1137	G
1	1	1142	A
1	1	1156	A
1	1	1169	A
1	1	1170	C
1	1	1173	U
1	1	1174	U
1	1	1175	A
1	1	1176	U
1	1	1178	C
1	1	1179	G
1	1	1180	U
1	1	1186	G
1	1	1206	G
1	1	1210	G
1	1	1227	G
1	1	1236	G
1	1	1238	G
1	1	1247	A
1	1	1248	G
1	1	1253	A
1	1	1256	G
1	1	1265	A
1	1	1266	G
1	1	1268	A
1	1	1271	G
1	1	1272	A
1	1	1273	U

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Mol	Chain	Res	Type
1	1	1275	A
1	1	1276	A
1	1	1287	A
1	1	1300	G
1	1	1301	A
1	1	1302	A
1	1	1321	A
1	1	1330	C
1	1	1345	C
1	1	1352	U
1	1	1363	C
1	1	1365	A
1	1	1368	G
1	1	1378	A
1	1	1379	U
1	1	1380	G
1	1	1383	A
1	1	1386	C
1	1	1387	A
1	1	1395	A
1	1	1406	U
1	1	1408	G
1	1	1409	U
1	1	1414	C
1	1	1415	U
1	1	1416	G
1	1	1417	C
1	1	1419	A
1	1	1420	A
1	1	1428	C
1	1	1434	A
1	1	1452	G
1	1	1453	A
1	1	1455	G
1	1	1459	G
1	1	1460	U
1	1	1478	G
1	1	1482	G
1	1	1490	A
1	1	1491	G
1	1	1493	C
1	1	1496	A

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Mol	Chain	Res	Type
1	1	1497	U
1	1	1498	C
1	1	1503	A
1	1	1508	A
1	1	1509	A
1	1	1510	G
1	1	1515	A
1	1	1520	U
1	1	1529	G
1	1	1534	U
1	1	1535	A
1	1	1536	C
1	1	1537	G
1	1	1554	U
1	1	1559	U
1	1	1566	A
1	1	1569	A
1	1	1570	A
1	1	1578	U
1	1	1580	A
1	1	1581	G
1	1	1583	A
1	1	1584	U
1	1	1589	U
1	1	1590	A
1	1	1593	A
1	1	1608	A
1	1	1609	A
1	1	1610	A
1	1	1613	G
1	1	1616	A
1	1	1618	6MZ
1	1	1647	U
1	1	1648	U
1	1	1649	G
1	1	1651	G
1	1	1654	A
1	1	1663	G
1	1	1664	A
1	1	1674	G
1	1	1677	A
1	1	1695	G

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Mol	Chain	Res	Type
1	1	1703	G
1	1	1713	A
1	1	1714	U
1	1	1715	G
1	1	1729	U
1	1	1730	C
1	1	1732	C
1	1	1733	G
1	1	1738	G
1	1	1742	U
1	1	1746	A
1	1	1750	G
1	1	1757	A
1	1	1758	U
1	1	1764	C
1	1	1773	A
1	1	1800	C
1	1	1801	A
1	1	1808	A
1	1	1811	G
1	1	1816	C
1	1	1829	A
1	1	1833	C
1	1	1842	G
1	1	1847	A
1	1	1848	A
1	1	1858	A
1	1	1859	U
1	1	1869	G
1	1	1870	C
1	1	1872	A
1	1	1873	G
1	1	1906	G
1	1	1907	G
1	1	1912	A
1	1	1913	A
1	1	1914	C
1	1	1916	A
1	1	1918	A
1	1	1919	A
1	1	1923	U
1	1	1924	C

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Mol	Chain	Res	Type
1	1	1929	G
1	1	1930	G
1	1	1936	A
1	1	1938	A
1	1	1939	5MU
1	1	1955	U
1	1	1960	A
1	1	1963	U
1	1	1967	C
1	1	1970	A
1	1	1971	U
1	1	1972	G
1	1	1982	U
1	1	1991	U
1	1	1992	G
1	1	1993	U
1	1	1997	C
1	1	2002	G
1	1	2020	A
1	1	2022	U
1	1	2023	C
1	1	2027	G
1	1	2031	A
1	1	2033	A
1	1	2043	C
1	1	2049	G
1	1	2051	A
1	1	2052	A
1	1	2055	C
1	1	2056	G
1	1	2060	A
1	1	2061	G
1	1	2062	A
1	1	2069	G7M
1	1	2077	A
1	1	2093	G
1	1	2097	A
1	1	2099	U
1	1	2100	G
1	1	2103	C
1	1	2107	G
1	1	2108	A

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Mol	Chain	Res	Type
1	1	2110	G
1	1	2111	U
1	1	2113	U
1	1	2115	G
1	1	2116	G
1	1	2117	A
1	1	2118	U
1	1	2121	G
1	1	2122	U
1	1	2124	G
1	1	2125	G
1	1	2126	A
1	1	2127	G
1	1	2128	G
1	1	2131	U
1	1	2132	U
1	1	2133	G
1	1	2134	A
1	1	2139	U
1	1	2141	G
1	1	2146	C
1	1	2147	A
1	1	2154	A
1	1	2157	G
1	1	2158	A
1	1	2159	G
1	1	2162	G
1	1	2163	A
1	1	2164	C
1	1	2165	C
1	1	2169	A
1	1	2171	A
1	1	2172	U
1	1	2178	C
1	1	2182	U
1	1	2183	A
1	1	2185	U
1	1	2186	G
1	1	2187	U
1	1	2188	U
1	1	2189	U
1	1	2193	G

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Mol	Chain	Res	Type
1	1	2194	U
1	1	2198	A
1	1	2203	U
1	1	2204	G
1	1	2209	G
1	1	2210	U
1	1	2211	A
1	1	2212	A
1	1	2213	U
1	1	2220	U
1	1	2225	A
1	1	2226	C
1	1	2229	U
1	1	2238	G
1	1	2239	G
1	1	2243	U
1	1	2244	U
1	1	2250	G
1	1	2251	OMG
1	1	2267	A
1	1	2268	A
1	1	2273	A
1	1	2275	C
1	1	2276	G
1	1	2278	A
1	1	2282	G
1	1	2283	C
1	1	2287	A
1	1	2288	A
1	1	2294	G
1	1	2297	A
1	1	2305	U
1	1	2308	G
1	1	2309	A
1	1	2311	A
1	1	2314	A
1	1	2322	A
1	1	2325	G
1	1	2327	A
1	1	2333	A
1	1	2334	U
1	1	2339	C

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Mol	Chain	Res	Type
1	1	2345	G
1	1	2347	C
1	1	2352	A
1	1	2361	G
1	1	2372	U
1	1	2376	A
1	1	2379	G
1	1	2382	G
1	1	2383	G
1	1	2385	C
1	1	2396	G
1	1	2402	U
1	1	2403	C
1	1	2406	A
1	1	2410	G
1	1	2423	U
1	1	2424	C
1	1	2425	A
1	1	2426	A
1	1	2429	G
1	1	2430	A
1	1	2431	U
1	1	2434	A
1	1	2435	A
1	1	2436	G
1	1	2441	U
1	1	2445	2MG
1	1	2448	A
1	1	2470	G
1	1	2473	U
1	1	2474	U
1	1	2476	A
1	1	2478	A
1	1	2491	U
1	1	2502	G
1	1	2505	G
1	1	2506	U
1	1	2507	C
1	1	2512	C
1	1	2513	A
1	1	2518	A
1	1	2520	C

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Mol	Chain	Res	Type
1	1	2525	G
1	1	2529	G
1	1	2534	A
1	1	2535	G
1	1	2547	A
1	1	2552	OMU
1	1	2554	U
1	1	2566	A
1	1	2567	G
1	1	2572	A
1	1	2573	C
1	1	2574	G
1	1	2585	U
1	1	2586	U
1	1	2602	A
1	1	2603	G
1	1	2609	U
1	1	2610	C
1	1	2611	C
1	1	2613	U
1	1	2623	G
1	1	2629	U
1	1	2663	G
1	1	2671	G
1	1	2689	U
1	1	2690	U
1	1	2714	G
1	1	2716	C
1	1	2722	G
1	1	2726	A
1	1	2733	A
1	1	2744	G
1	1	2748	A
1	1	2751	G
1	1	2757	A
1	1	2758	A
1	1	2762	C
1	1	2765	A
1	1	2777	G
1	1	2791	G
1	1	2796	U
1	1	2797	U

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Mol	Chain	Res	Type
1	1	2798	U
1	1	2799	A
1	1	2801	G
1	1	2818	U
1	1	2820	A
1	1	2821	A
1	1	2824	C
1	1	2825	G
1	1	2849	U
1	1	2854	G
1	1	2859	G
1	1	2861	U
1	1	2867	G
1	1	2880	C
1	1	2883	A
1	1	2884	U
1	1	2891	U
1	1	2902	C
2	2	4	U
2	2	5	U
2	2	8	A
2	2	9	G
2	2	22	G
2	2	29	U
2	2	32	A
2	2	38	G
2	2	39	G
2	2	41	G
2	2	47	C
2	2	48	C
2	2	51	A
2	2	52	C
2	2	54	C
2	2	58	C
2	2	68	G
2	2	69	G
2	2	70	U
2	2	71	A
2	2	72	A
2	2	74	A
2	2	76	G
2	2	82	G

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Mol	Chain	Res	Type
2	2	83	C
2	2	84	U
2	2	87	C
2	2	90	C
2	2	94	G
2	2	95	C
2	2	96	U
2	2	108	G
2	2	116	A
2	2	120	A
2	2	121	U
2	2	122	G
2	2	128	G
2	2	131	A
2	2	141	G
2	2	144	G
2	2	147	G
2	2	149	A
2	2	160	A
2	2	161	A
2	2	164	G
2	2	173	U
2	2	174	A
2	2	181	A
2	2	182	A
2	2	196	A
2	2	197	A
2	2	198	G
2	2	204	G
2	2	208	U
2	2	209	U
2	2	210	C
2	2	211	G
2	2	212	G
2	2	214	C
2	2	226	G
2	2	245	U
2	2	247	G
2	2	251	G
2	2	262	A
2	2	266	G
2	2	267	C

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Mol	Chain	Res	Type
2	2	271	C
2	2	279	A
2	2	280	C
2	2	289	G
2	2	299	G
2	2	306	A
2	2	316	C
2	2	319	G
2	2	321	A
2	2	328	C
2	2	329	A
2	2	332	G
2	2	341	C
2	2	347	G
2	2	352	C
2	2	354	G
2	2	355	C
2	2	367	U
2	2	372	C
2	2	373	A
2	2	376	G
2	2	382	A
2	2	384	G
2	2	388	G
2	2	389	A
2	2	392	C
2	2	393	A
2	2	397	A
2	2	406	G
2	2	411	A
2	2	412	A
2	2	413	G
2	2	414	A
2	2	421	U
2	2	422	C
2	2	424	G
2	2	429	U
2	2	436	C
2	2	439	U
2	2	446	G
2	2	451	A
2	2	457	G

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Mol	Chain	Res	Type
2	2	458	U
2	2	460	A
2	2	463	U
2	2	464	U
2	2	467	U
2	2	468	A
2	2	469	C
2	2	478	A
2	2	479	U
2	2	480	U
2	2	481	G
2	2	484	G
2	2	485	U
2	2	486	U
2	2	495	A
2	2	496	A
2	2	497	G
2	2	511	C
2	2	514	C
2	2	517	G
2	2	518	C
2	2	519	C
2	2	523	A
2	2	526	C
2	2	527	7MG
2	2	528	C
2	2	531	U
2	2	532	A
2	2	533	A
2	2	536	C
2	2	537	G
2	2	539	A
2	2	547	A
2	2	559	A
2	2	567	G
2	2	568	G
2	2	570	G
2	2	572	A
2	2	573	A
2	2	576	C
2	2	577	G
2	2	579	A

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Mol	Chain	Res	Type
2	2	596	A
2	2	607	A
2	2	628	G
2	2	633	G
2	2	641	U
2	2	642	A
2	2	649	A
2	2	650	G
2	2	653	U
2	2	654	G
2	2	665	A
2	2	700	G
2	2	702	A
2	2	705	G
2	2	723	U
2	2	724	G
2	2	731	G
2	2	734	G
2	2	742	G
2	2	747	A
2	2	748	G
2	2	755	G
2	2	760	G
2	2	777	A
2	2	793	U
2	2	794	A
2	2	799	G
2	2	802	A
2	2	813	U
2	2	814	A
2	2	815	A
2	2	817	C
2	2	828	U
2	2	832	G
2	2	841	C
2	2	844	G
2	2	845	A
2	2	846	G
2	2	849	G
2	2	872	A
2	2	874	G
2	2	876	C

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Mol	Chain	Res	Type
2	2	885	G
2	2	887	G
2	2	902	G
2	2	914	A
2	2	916	U
2	2	928	G
2	2	934	C
2	2	935	A
2	2	936	C
2	2	945	G
2	2	958	A
2	2	960	U
2	2	966	2MG
2	2	967	5MC
2	2	968	A
2	2	969	A
2	2	972	C
2	2	975	A
2	2	976	G
2	2	978	A
2	2	984	C
2	2	987	G
2	2	989	U
2	2	991	U
2	2	992	U
2	2	993	G
2	2	996	A
2	2	1004	A
2	2	1005	A
2	2	1008	U
2	2	1009	U
2	2	1017	U
2	2	1018	G
2	2	1021	A
2	2	1024	G
2	2	1026	G
2	2	1028	C
2	2	1030	U
2	2	1031	C
2	2	1037	C
2	2	1042	A
2	2	1043	G

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Mol	Chain	Res	Type
2	2	1044	A
2	2	1046	A
2	2	1065	U
2	2	1074	G
2	2	1085	U
2	2	1094	G
2	2	1095	U
2	2	1099	G
2	2	1101	A
2	2	1124	G
2	2	1133	G
2	2	1135	U
2	2	1136	C
2	2	1137	C
2	2	1139	G
2	2	1140	C
2	2	1141	C
2	2	1142	G
2	2	1143	G
2	2	1146	A
2	2	1151	A
2	2	1152	A
2	2	1159	U
2	2	1160	G
2	2	1167	A
2	2	1171	A
2	2	1174	G
2	2	1175	G
2	2	1176	A
2	2	1184	G
2	2	1196	A
2	2	1197	A
2	2	1200	C
2	2	1206	G
2	2	1211	U
2	2	1212	U
2	2	1213	A
2	2	1214	C
2	2	1215	G
2	2	1225	A
2	2	1226	C
2	2	1227	A

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Mol	Chain	Res	Type
2	2	1228	C
2	2	1238	A
2	2	1239	A
2	2	1248	A
2	2	1256	A
2	2	1257	A
2	2	1275	A
2	2	1278	G
2	2	1279	G
2	2	1280	A
2	2	1285	A
2	2	1286	U
2	2	1287	A
2	2	1299	A
2	2	1300	G
2	2	1302	C
2	2	1305	G
2	2	1312	G
2	2	1317	C
2	2	1320	C
2	2	1332	A
2	2	1338	G
2	2	1340	A
2	2	1346	A
2	2	1347	G
2	2	1348	U
2	2	1353	G
2	2	1363	A
2	2	1370	G
2	2	1378	C
2	2	1379	G
2	2	1381	U
2	2	1383	C
2	2	1396	A
2	2	1397	C
2	2	1402	4OC
2	2	1403	C
2	2	1404	C
2	2	1414	U
2	2	1419	G
2	2	1429	A
2	2	1441	A

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Mol	Chain	Res	Type
2	2	1446	A
2	2	1447	A
2	2	1448	C
2	2	1452	C
2	2	1453	G
2	2	1475	G
2	2	1480	A
2	2	1492	A
2	2	1494	G
2	2	1497	G
2	2	1499	A
2	2	1503	A
2	2	1506	U
2	2	1516	2MG
2	2	1517	G
2	2	1529	G
2	2	1530	G
2	2	1534	A
3	3	2	G
3	3	15	A
3	3	16	G
3	3	17	C
3	3	21	G
3	3	35	C
3	3	36	C
3	3	45	A
3	3	51	G
3	3	56	G
3	3	64	G
3	3	66	A
3	3	67	G
3	3	88	C
3	3	89	U
3	3	90	C
3	3	99	A
3	3	105	G
3	3	109	A
3	3	120	U
4	4	15	A
5	5	3	G
5	5	5	G
5	5	8	4SU

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Mol	Chain	Res	Type
5	5	9	G
5	5	13	A
5	5	15	C
5	5	16	C
5	5	17	U
5	5	18	G
5	5	19	G
5	5	20	H2U
5	5	21	A
5	5	22	G
5	5	25	C
5	5	31	G
5	5	47	U
5	5	48	C
5	5	49	G
5	5	55	PSU
5	5	56	C
5	5	57	A
5	5	59	A
5	5	69	C
5	5	74	C

All (138) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	62	U
1	1	101	A
1	1	138	U
1	1	140	C
1	1	196	A
1	1	199	A
1	1	271	G
1	1	369	U
1	1	404	A
1	1	446	G
1	1	503	A
1	1	546	U
1	1	548	G
1	1	571	U
1	1	573	U
1	1	603	A
1	1	614	A

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Mol	Chain	Res	Type
1	1	620	G
1	1	682	G
1	1	752	A
1	1	764	A
1	1	784	G
1	1	805	G
1	1	883	G
1	1	892	A
1	1	894	U
1	1	895	U
1	1	896	A
1	1	984	A
1	1	995	C
1	1	1061	U
1	1	1063	G
1	1	1064	C
1	1	1070	A
1	1	1082	U
1	1	1094	U
1	1	1109	C
1	1	1110	G
1	1	1128	G
1	1	1133	A
1	1	1142	A
1	1	1173	U
1	1	1253	A
1	1	1272	A
1	1	1275	A
1	1	1320	C
1	1	1344	U
1	1	1379	U
1	1	1395	A
1	1	1396	U
1	1	1415	U
1	1	1490	A
1	1	1497	U
1	1	1509	A
1	1	1583	A
1	1	1584	U
1	1	1608	A
1	1	1647	U
1	1	1913	A

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Mol	Chain	Res	Type
1	1	1918	A
1	1	1923	U
1	1	1962	5MC
1	1	2062	A
1	1	2146	C
1	1	2162	G
1	1	2193	G
1	1	2210	U
1	1	2211	A
1	1	2212	A
1	1	2225	A
1	1	2244	U
1	1	2250	G
1	1	2275	C
1	1	2282	G
1	1	2296	U
1	1	2324	U
1	1	2326	C
1	1	2382	G
1	1	2425	A
1	1	2447	G
1	1	2473	U
1	1	2506	U
1	1	2572	A
1	1	2602	A
1	1	2610	C
1	1	2756	U
1	1	2796	U
1	1	2797	U
1	1	2798	U
1	1	2820	A
1	1	2873	A
2	2	70	U
2	2	121	U
2	2	181	A
2	2	183	C
2	2	197	A
2	2	209	U
2	2	305	G
2	2	421	U
2	2	428	G
2	2	429	U

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Mol	Chain	Res	Type
2	2	481	G
2	2	496	A
2	2	517	G
2	2	531	U
2	2	559	A
2	2	575	G
2	2	641	U
2	2	653	U
2	2	702	A
2	2	733	G
2	2	793	U
2	2	966	2MG
2	2	967	5MC
2	2	991	U
2	2	992	U
2	2	1145	A
2	2	1196	A
2	2	1212	U
2	2	1213	A
2	2	1214	C
2	2	1225	A
2	2	1299	A
2	2	1346	A
2	2	1363	A
2	2	1396	A
2	2	1403	C
2	2	1407	5MC
2	2	1447	A
2	2	1516	2MG
3	3	48	U
5	5	8	4SU
5	5	16	C
5	5	17	U
5	5	18	G
5	5	19	G
5	5	47	U
5	5	60	U

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	PSU	1	1917	1	18,21,22	1.23	2 (11%)	22,30,33	1.34	4 (18%)
1	5MU	1	1939	1	19,22,23	0.79	1 (5%)	28,32,35	1.05	3 (10%)
5	8AN	5	76	59,60,1,5	22,24,25	0.38	0	26,35,38	0.38	0
5	4SU	5	8	5	18,21,22	1.55	3 (16%)	26,30,33	2.78	12 (46%)
2	5MC	2	1407	2	18,22,23	0.84	1 (5%)	26,32,35	1.29	3 (11%)
2	2MG	2	1516	2	23,26,27	0.64	0	32,38,41	1.23	2 (6%)
1	OMG	1	2251	1,5	23,26,27	0.90	2 (8%)	33,38,41	2.37	4 (12%)
1	6MZ	1	2030	1	22,25,26	0.73	0	30,36,39	1.73	6 (20%)
49	0TD	q	89	49	7,9,10	6.74	5 (71%)	6,11,13	4.11	2 (33%)
1	OMU	1	2552	1	19,22,23	0.53	0	26,31,34	0.81	1 (3%)
2	7MG	2	527	2	22,26,27	1.46	4 (18%)	29,39,42	2.99	10 (34%)
5	PSU	5	55	5	18,21,22	1.79	1 (5%)	22,30,33	1.60	3 (13%)
1	2MG	1	1835	1	23,26,27	0.62	0	32,38,41	1.21	3 (9%)
1	2MG	1	2445	1	23,26,27	0.76	0	32,38,41	1.05	2 (6%)
1	6MZ	1	1618	1	22,25,26	0.63	0	30,36,39	1.44	3 (10%)
5	H2U	5	20	5	18,21,22	0.65	0	21,30,33	1.92	4 (19%)
1	PSU	1	2457	1	18,21,22	2.22	1 (5%)	22,30,33	1.42	4 (18%)
2	UR3	2	1498	2	19,22,23	0.81	0	26,32,35	1.02	1 (3%)
2	PSU	2	516	59,2	18,21,22	1.55	1 (5%)	22,30,33	1.62	2 (9%)
1	G7M	1	2069	1	23,26,27	1.11	2 (8%)	35,39,42	1.98	6 (17%)
2	5MC	2	967	2	18,22,23	0.76	1 (5%)	26,32,35	1.30	3 (11%)
2	2MG	2	966	2	23,26,27	0.61	0	32,38,41	1.49	3 (9%)
1	1MG	1	745	1	22,26,27	1.11	2 (9%)	33,39,42	1.60	5 (15%)
1	PSU	1	2580	1	18,21,22	1.88	1 (5%)	22,30,33	1.37	3 (13%)
1	5MU	1	747	1	19,22,23	0.75	1 (5%)	28,32,35	1.08	4 (14%)
1	OMC	1	2498	59,1	19,22,23	1.17	2 (10%)	26,31,34	1.61	3 (11%)
1	2MA	1	2503	59,1	22,25,26	1.41	4 (18%)	33,37,40	2.55	13 (39%)
1	PSU	1	955	1	18,21,22	1.87	1 (5%)	22,30,33	1.66	3 (13%)
1	PSU	1	2605	1	18,21,22	1.90	1 (5%)	22,30,33	1.69	3 (13%)
2	MA6	2	1518	2	23,26,27	0.55	0	34,38,41	1.10	3 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	4OC	5	32	5	20,23,24	0.58	0	26,32,35	1.23	2 (7%)
1	PSU	1	1911	1	18,21,22	0.83	1 (5%)	22,30,33	1.11	2 (9%)
2	2MG	2	1207	2	23,26,27	0.94	0	32,38,41	0.85	1 (3%)
1	PSU	1	746	59,1	18,21,22	2.01	1 (5%)	22,30,33	2.10	3 (13%)
1	3TD	1	1915	1	18,22,23	2.41	6 (33%)	22,32,35	1.85	4 (18%)
5	5MU	5	54	5	19,22,23	0.67	0	28,32,35	0.97	2 (7%)
1	PSU	1	2504	1	18,21,22	1.86	1 (5%)	22,30,33	1.64	3 (13%)
2	MA6	2	1519	2	23,26,27	0.63	0	34,38,41	1.11	3 (8%)
2	4OC	2	1402	2	20,23,24	0.68	0	26,32,35	1.59	3 (11%)
1	5MC	1	1962	1	18,22,23	0.85	1 (5%)	26,32,35	1.52	3 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1	1917	1	-	0/7/25/26	0/2/2/2
1	5MU	1	1939	1	-	0/7/25/26	0/2/2/2
5	8AN	5	76	59,60,1,5	-	1/7/25/26	0/3/3/3
5	4SU	5	8	5	-	3/7/25/26	0/2/2/2
2	5MC	2	1407	2	-	0/7/25/26	0/2/2/2
2	2MG	2	1516	2	-	0/9/27/28	0/3/3/3
1	OMG	1	2251	1,5	-	4/9/27/28	0/3/3/3
1	6MZ	1	2030	1	-	1/9/27/28	0/3/3/3
49	0TD	q	89	49	-	2/7/12/14	-
1	OMU	1	2552	1	-	2/9/27/28	0/2/2/2
2	7MG	2	527	2	-	3/7/37/38	0/3/3/3
5	PSU	5	55	5	-	3/7/25/26	0/2/2/2
1	2MG	1	1835	1	-	2/9/27/28	0/3/3/3
1	2MG	1	2445	1	-	2/9/27/28	0/3/3/3
1	6MZ	1	1618	1	-	5/9/27/28	0/3/3/3
5	H2U	5	20	5	-	4/7/38/39	0/2/2/2
1	PSU	1	2457	1	-	1/7/25/26	0/2/2/2
2	UR3	2	1498	2	-	0/7/25/26	0/2/2/2
2	PSU	2	516	59,2	-	2/7/25/26	0/2/2/2
1	G7M	1	2069	1	-	2/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5MC	2	967	2	-	5/7/25/26	0/2/2/2
2	2MG	2	966	2	-	6/9/27/28	0/3/3/3
1	1MG	1	745	1	-	2/7/25/26	0/3/3/3
1	PSU	1	2580	1	-	2/7/25/26	0/2/2/2
1	5MU	1	747	1	-	0/7/25/26	0/2/2/2
1	OMC	1	2498	59,1	-	2/9/27/28	0/2/2/2
1	2MA	1	2503	59,1	-	2/7/25/26	0/3/3/3
1	PSU	1	955	1	-	0/7/25/26	0/2/2/2
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2
2	MA6	2	1518	2	-	0/11/29/30	0/3/3/3
5	4OC	5	32	5	-	0/9/29/30	0/2/2/2
1	PSU	1	1911	1	-	0/7/25/26	0/2/2/2
2	2MG	2	1207	2	-	0/9/27/28	0/3/3/3
1	PSU	1	746	59,1	-	2/7/25/26	0/2/2/2
1	3TD	1	1915	1	-	2/7/25/26	0/2/2/2
5	5MU	5	54	5	-	0/7/25/26	0/2/2/2
1	PSU	1	2504	1	-	1/7/25/26	0/2/2/2
2	MA6	2	1519	2	-	6/11/29/30	0/3/3/3
2	4OC	2	1402	2	-	1/9/29/30	0/2/2/2
1	5MC	1	1962	1	-	1/7/25/26	0/2/2/2

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	q	89	0TD	CB-SB	-16.93	1.65	1.82
1	1	2457	PSU	C2'-C1'	-9.03	1.42	1.53
1	1	746	PSU	C2'-C1'	-8.32	1.42	1.53
1	1	2605	PSU	C2'-C1'	-7.74	1.43	1.53
1	1	2504	PSU	C2'-C1'	-7.60	1.43	1.53
1	1	2580	PSU	C2'-C1'	-7.58	1.43	1.53
5	5	55	PSU	C2'-C1'	-7.36	1.44	1.53
1	1	955	PSU	C2'-C1'	-7.21	1.44	1.53
2	2	516	PSU	C2'-C1'	-6.32	1.45	1.53
1	1	1915	3TD	C1'-C5	-6.19	1.36	1.50
1	1	1915	3TD	C6-C5	-5.83	1.28	1.35
5	5	8	4SU	C4-S4	-4.52	1.59	1.68
1	1	2498	OMC	C3'-C2'	-3.75	1.44	1.52
1	1	2503	2MA	C2-N1	3.68	1.40	1.34
2	2	527	7MG	C4-N9	-3.41	1.33	1.37
49	q	89	0TD	CA-N	-3.17	1.37	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2069	G7M	C2'-C1'	-3.06	1.43	1.53
1	1	2503	2MA	C6-N1	3.03	1.39	1.35
1	1	1915	3TD	O5'-C5'	2.87	1.51	1.44
1	1	745	1MG	C5-C6	-2.84	1.38	1.45
1	1	1915	3TD	O2-C2	-2.83	1.17	1.23
1	1	1915	3TD	C4-N3	-2.73	1.34	1.40
5	5	8	4SU	C5-C4	-2.71	1.39	1.42
1	1	1962	5MC	C2'-C1'	-2.71	1.44	1.53
49	q	89	0TD	OD2-CG	-2.70	1.21	1.30
49	q	89	0TD	CB-CG	-2.68	1.47	1.52
1	1	745	1MG	C2'-C1'	-2.65	1.45	1.53
2	2	527	7MG	C6-N1	-2.63	1.34	1.38
1	1	2503	2MA	C6-N6	-2.63	1.27	1.34
1	1	1911	PSU	C2'-C1'	-2.57	1.50	1.53
2	2	527	7MG	C5-C4	2.54	1.46	1.38
49	q	89	0TD	CSB-SB	-2.53	1.74	1.79
1	1	1939	5MU	C2'-C1'	-2.52	1.45	1.53
1	1	2069	G7M	O2'-C2'	-2.52	1.37	1.43
1	1	2498	OMC	C2'-C1'	-2.49	1.46	1.53
5	5	8	4SU	C2-N1	2.46	1.42	1.38
1	1	2251	OMG	C2'-C1'	-2.45	1.46	1.53
2	2	527	7MG	C5-N7	-2.39	1.32	1.35
1	1	2503	2MA	C2'-C3'	-2.38	1.46	1.53
1	1	747	5MU	C2'-C1'	-2.29	1.46	1.53
1	1	2251	OMG	C3'-C2'	-2.27	1.47	1.52
1	1	1917	PSU	C2'-C1'	-2.19	1.50	1.53
2	2	967	5MC	C2'-C1'	-2.10	1.46	1.53
1	1	1917	PSU	C6-N1	-2.06	1.32	1.36
2	2	1407	5MC	C2'-C1'	-2.05	1.46	1.53
1	1	1915	3TD	C2-N1	2.01	1.39	1.37

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2251	OMG	O2'-C2'-C1'	10.32	129.21	109.08
2	2	527	7MG	N9-C4-N3	9.24	139.29	125.47
1	1	746	PSU	C3'-C2'-C1'	7.62	110.52	101.64
49	q	89	0TD	CB-CA-N	-7.52	93.08	109.10
1	1	2503	2MA	C3'-C2'-C1'	-7.06	88.01	101.43
1	1	1915	3TD	C6-C5-C4	6.86	122.96	118.22
5	5	8	4SU	C5-C4-S4	-6.64	115.91	124.47
2	2	1402	4OC	O3'-C3'-C2'	6.64	130.03	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	8	4SU	C5-C4-N3	6.64	120.84	114.69
5	5	8	4SU	C4-N3-C2	-6.42	121.11	127.34
1	1	2498	OMC	O3'-C3'-C2'	6.40	129.33	111.17
2	2	966	2MG	O3'-C3'-C4'	6.30	129.27	111.05
49	q	89	0TD	CSB-SB-CB	6.19	113.63	102.44
2	2	527	7MG	O4'-C1'-N9	5.92	117.36	109.30
1	1	1962	5MC	O3'-C3'-C4'	5.75	127.66	111.05
2	2	527	7MG	N9-C8-N7	-5.72	95.19	103.38
2	2	527	7MG	C5-C4-N3	-5.56	117.53	128.13
2	2	516	PSU	O2'-C2'-C3'	5.48	129.56	111.82
1	1	745	1MG	O3'-C3'-C4'	5.44	126.77	111.05
1	1	1618	6MZ	O3'-C3'-C4'	5.37	126.56	111.05
1	1	2503	2MA	O3'-C3'-C2'	5.28	128.91	111.82
1	1	2251	OMG	O3'-C3'-C2'	5.27	126.12	111.17
1	1	2503	2MA	O2'-C2'-C1'	5.23	127.50	110.02
2	2	1516	2MG	O3'-C3'-C2'	5.19	128.59	111.82
5	5	55	PSU	O2'-C2'-C3'	5.05	128.14	111.82
1	1	2069	G7M	C2'-C1'-N9	5.02	127.43	113.22
1	1	2251	OMG	O3'-C3'-C4'	4.99	125.47	111.05
1	1	2030	6MZ	C3'-C2'-C1'	-4.98	91.96	101.43
1	1	2030	6MZ	O3'-C3'-C4'	4.92	125.28	111.05
1	1	2504	PSU	O2'-C2'-C3'	4.77	127.27	111.82
1	1	2069	G7M	O2'-C2'-C1'	4.73	125.83	110.02
1	1	2605	PSU	O2'-C2'-C3'	4.69	127.00	111.82
1	1	2069	G7M	C4'-O4'-C1'	-4.69	99.12	109.47
1	1	955	PSU	O2'-C2'-C3'	4.65	126.86	111.82
5	5	20	H2U	O2'-C2'-C3'	4.63	126.79	111.82
1	1	745	1MG	C3'-C2'-C1'	4.62	110.21	101.43
1	1	2605	PSU	O2'-C2'-C1'	4.59	122.17	111.23
2	2	527	7MG	C2-N3-C4	4.58	120.46	112.30
2	2	1407	5MC	O3'-C3'-C2'	4.46	126.24	111.82
1	1	955	PSU	O2'-C2'-C1'	4.40	121.71	111.23
5	5	20	H2U	O3'-C3'-C4'	4.39	123.73	111.05
1	1	2503	2MA	C4'-O4'-C1'	-4.38	99.81	109.47
1	1	746	PSU	O2'-C2'-C3'	4.21	125.46	111.82
1	1	2069	G7M	O2'-C2'-C3'	4.18	125.33	111.82
5	5	20	H2U	O3'-C3'-C2'	4.15	125.24	111.82
1	1	2498	OMC	O2'-C2'-C1'	4.09	117.07	109.08
1	1	1835	2MG	O3'-C3'-C4'	4.06	122.79	111.05
1	1	2504	PSU	O2'-C2'-C1'	4.05	120.89	111.23
1	1	2457	PSU	O2'-C2'-C3'	3.92	124.52	111.82
5	5	55	PSU	O2'-C2'-C1'	3.91	120.55	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	32	4OC	O3'-C3'-C2'	3.85	122.10	111.17
1	1	2580	PSU	O2'-C2'-C3'	3.85	124.27	111.82
1	1	2503	2MA	O3'-C3'-C4'	3.84	122.17	111.05
5	5	8	4SU	C1'-N1-C2	3.83	124.50	117.57
2	2	1518	MA6	C2-N1-C6	3.70	120.48	111.75
2	2	967	5MC	O3'-C3'-C2'	3.69	123.77	111.82
1	1	2069	G7M	C3'-C2'-C1'	-3.68	94.44	101.43
5	5	20	H2U	O2'-C2'-C1'	3.62	122.14	110.02
1	1	2251	OMG	C3'-C2'-C1'	3.62	109.69	102.89
2	2	516	PSU	O2'-C2'-C1'	3.53	119.66	111.23
1	1	1939	5MU	C2'-C1'-N1	3.46	123.03	113.22
1	1	2580	PSU	O2'-C2'-C1'	3.40	119.33	111.23
1	1	2445	2MG	O3'-C3'-C2'	3.34	122.61	111.82
2	2	966	2MG	C2'-C3'-C4'	-3.29	96.26	102.64
1	1	745	1MG	O3'-C3'-C2'	3.28	122.44	111.82
1	1	2503	2MA	O4'-C1'-N9	-3.26	101.63	108.06
2	2	1518	MA6	C4-N9-C8	3.26	109.26	105.73
2	2	1519	MA6	C4-N9-C8	3.25	109.25	105.73
5	5	8	4SU	N3-C2-N1	3.24	119.19	114.89
1	1	746	PSU	O2'-C2'-C1'	3.24	118.95	111.23
2	2	1519	MA6	C2-N1-C6	3.23	119.38	111.75
2	2	1516	2MG	O3'-C3'-C4'	3.19	120.28	111.05
1	1	2030	6MZ	C4-N9-C8	3.19	109.18	105.73
1	1	2503	2MA	O2'-C2'-C3'	3.18	122.09	111.82
1	1	1917	PSU	C3'-C2'-C1'	3.16	105.32	101.64
1	1	2504	PSU	C2'-C3'-C4'	-3.16	96.51	102.64
1	1	1618	6MZ	C4-N9-C8	3.11	109.10	105.73
5	5	8	4SU	S4-C4-N3	3.09	123.25	120.21
1	1	2457	PSU	O2'-C2'-C1'	3.07	118.55	111.23
1	1	1835	2MG	O3'-C3'-C2'	3.05	121.70	111.82
2	2	967	5MC	O3'-C3'-C4'	3.02	119.79	111.05
2	2	527	7MG	C5-C6-N1	3.01	116.30	110.99
1	1	1618	6MZ	C2'-C1'-N9	2.99	120.88	113.30
2	2	1498	UR3	O4'-C1'-C2'	-2.99	100.13	106.64
1	1	955	PSU	C2'-C3'-C4'	-2.98	96.84	102.64
5	5	55	PSU	C3'-C2'-C1'	2.97	105.09	101.64
1	1	2503	2MA	C4-N9-C8	2.93	108.90	105.73
1	1	2445	2MG	O3'-C3'-C4'	2.92	119.48	111.05
5	5	32	4OC	O3'-C3'-C4'	2.91	119.46	111.05
2	2	527	7MG	O4'-C4'-C3'	-2.89	99.39	105.11
1	1	1915	3TD	O4'-C4'-C5'	-2.89	99.86	109.37
1	1	2503	2MA	O4'-C1'-C2'	2.87	112.90	106.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1911	PSU	C3'-C2'-C1'	2.81	104.91	101.64
1	1	2030	6MZ	C4'-O4'-C1'	-2.81	103.28	109.47
1	1	747	5MU	C2'-C1'-N1	2.77	121.06	113.22
5	5	8	4SU	C2'-C1'-N1	2.70	120.87	113.22
2	2	1402	4OC	O3'-C3'-C4'	2.67	118.78	111.05
1	1	1917	PSU	O2-C2-N1	-2.67	119.85	122.79
1	1	2069	G7M	C2'-C3'-C4'	-2.64	97.51	102.64
1	1	2457	PSU	C3'-C2'-C1'	2.63	104.69	101.64
1	1	2605	PSU	C2'-C3'-C4'	-2.62	97.56	102.64
2	2	1402	4OC	O4'-C4'-C3'	-2.58	100.00	105.11
5	5	54	5MU	C2'-C1'-N1	2.57	120.50	113.22
2	2	1518	MA6	C2'-C3'-C4'	-2.56	97.66	102.64
1	1	2030	6MZ	O3'-C3'-C2'	2.56	120.10	111.82
2	2	966	2MG	O3'-C3'-C2'	2.53	119.99	111.82
1	1	2503	2MA	C5-C4-N3	-2.51	124.36	127.19
1	1	1962	5MC	O3'-C3'-C2'	2.51	119.95	111.82
2	2	527	7MG	C5-C4-N9	-2.46	103.16	106.35
1	1	1835	2MG	C3'-C2'-C1'	2.44	106.06	101.43
2	2	967	5MC	C2'-C1'-N1	2.40	120.02	113.22
1	1	2580	PSU	C3'-C2'-C1'	2.39	104.42	101.64
1	1	745	1MG	O2'-C2'-C1'	2.37	117.93	110.02
1	1	2457	PSU	C2'-C3'-C4'	-2.36	98.05	102.64
2	2	527	7MG	O6-C6-C5	-2.35	121.76	127.54
1	1	1917	PSU	N1-C2-N3	2.34	117.78	115.13
1	1	2503	2MA	N3-C4-N9	2.32	130.22	126.99
1	1	1911	PSU	O3'-C3'-C4'	2.31	117.72	111.05
2	2	1407	5MC	C2'-C1'-N1	2.24	119.58	113.22
2	2	1207	2MG	O2'-C2'-C1'	-2.24	102.52	110.02
1	1	747	5MU	C3'-C2'-C1'	2.24	105.68	101.43
1	1	2503	2MA	C1'-N9-C8	-2.22	122.12	127.14
2	2	1407	5MC	O3'-C3'-C4'	2.20	117.42	111.05
1	1	1939	5MU	N3-C2-N1	2.20	117.81	114.89
2	2	1519	MA6	C2'-C3'-C4'	-2.20	98.36	102.64
1	1	1939	5MU	C4-N3-C2	-2.20	124.51	127.35
1	1	2503	2MA	N9-C8-N7	-2.16	110.96	113.91
1	1	2552	OMU	N3-C2-N1	2.15	117.75	114.89
1	1	747	5MU	N3-C2-N1	2.15	117.74	114.89
1	1	1917	PSU	C6-C5-C4	2.14	119.69	118.20
5	5	54	5MU	N3-C2-N1	2.13	117.72	114.89
1	1	747	5MU	C4-N3-C2	-2.12	124.61	127.35
5	5	8	4SU	C4'-O4'-C1'	-2.11	104.81	109.47
1	1	1915	3TD	C3'-C2'-C1'	2.11	104.09	101.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1962	5MC	C3'-C2'-C1'	2.11	105.43	101.43
5	5	8	4SU	O4'-C1'-C2'	-2.10	102.07	106.64
1	1	745	1MG	O2'-C2'-C3'	2.09	118.59	111.82
5	5	8	4SU	C1'-N1-C6	-2.09	116.29	120.84
5	5	8	4SU	O2-C2-N1	-2.07	120.04	122.79
1	1	2498	OMC	C3'-C2'-C1'	2.03	106.71	102.89
1	1	2030	6MZ	C2'-C1'-N9	2.03	118.43	113.30
1	1	1915	3TD	C4-N3-C2	-2.01	122.43	124.61
2	2	527	7MG	O2'-C2'-C1'	-2.01	103.32	110.02
5	5	8	4SU	C6-C5-C4	-2.00	118.22	119.95

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	746	PSU	C2'-C1'-C5-C4
1	1	1618	6MZ	N1-C6-N6-C9
1	1	1618	6MZ	O4'-C4'-C5'-O5'
1	1	1618	6MZ	C3'-C4'-C5'-O5'
1	1	1835	2MG	N1-C2-N2-CM2
1	1	1835	2MG	N3-C2-N2-CM2
1	1	1915	3TD	O4'-C1'-C5-C4
1	1	1915	3TD	O4'-C1'-C5-C6
1	1	2069	G7M	O4'-C4'-C5'-O5'
1	1	2251	OMG	C1'-C2'-O2'-CM2
1	1	2445	2MG	C3'-C4'-C5'-O5'
2	2	966	2MG	O4'-C4'-C5'-O5'
2	2	966	2MG	C3'-C4'-C5'-O5'
2	2	966	2MG	N1-C2-N2-CM2
2	2	966	2MG	N3-C2-N2-CM2
2	2	967	5MC	O4'-C4'-C5'-O5'
2	2	1519	MA6	C5-C6-N6-C10
5	5	20	H2U	O4'-C4'-C5'-O5'
5	5	20	H2U	O4'-C1'-N1-C6
5	5	55	PSU	C3'-C4'-C5'-O5'
49	q	89	0TD	SB-CB-CG-OD2
2	2	967	5MC	C3'-C4'-C5'-O5'
2	2	1519	MA6	O4'-C4'-C5'-O5'
5	5	20	H2U	C3'-C4'-C5'-O5'
1	1	2552	OMU	O4'-C4'-C5'-O5'
2	2	1519	MA6	C3'-C4'-C5'-O5'
5	5	20	H2U	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
2	2	1519	MA6	N1-C6-N6-C10
1	1	745	1MG	O4'-C4'-C5'-O5'
1	1	745	1MG	C3'-C4'-C5'-O5'
2	2	527	7MG	C3'-C4'-C5'-O5'
1	1	2552	OMU	C3'-C4'-C5'-O5'
5	5	55	PSU	O4'-C4'-C5'-O5'
1	1	2445	2MG	O4'-C4'-C5'-O5'
1	1	2498	OMC	O4'-C4'-C5'-O5'
2	2	527	7MG	O4'-C4'-C5'-O5'
5	5	76	8AN	C4'-C5'-O5'-P
2	2	1519	MA6	C5-C6-N6-C9
1	1	2498	OMC	C3'-C4'-C5'-O5'
2	2	516	PSU	O4'-C4'-C5'-O5'
1	1	1618	6MZ	C5-C6-N6-C9
49	q	89	0TD	CG-CB-SB-CSB
5	5	8	4SU	O4'-C1'-N1-C6
5	5	8	4SU	O4'-C1'-N1-C2
1	1	2069	G7M	C4'-C5'-O5'-P
2	2	967	5MC	C4'-C5'-O5'-P
1	1	2251	OMG	O4'-C4'-C5'-O5'
2	2	1402	4OC	O4'-C4'-C5'-O5'
2	2	527	7MG	C4'-C5'-O5'-P
2	2	1519	MA6	C4'-C5'-O5'-P
1	1	2457	PSU	O4'-C1'-C5-C4
1	1	2580	PSU	O4'-C1'-C5-C4
1	1	2251	OMG	C3'-C2'-O2'-CM2
2	2	967	5MC	C2'-C1'-N1-C6
1	1	2251	OMG	C3'-C4'-C5'-O5'
1	1	2503	2MA	O4'-C4'-C5'-O5'
1	1	2503	2MA	O4'-C1'-N9-C8
1	1	2504	PSU	O4'-C4'-C5'-O5'
2	2	516	PSU	C3'-C4'-C5'-O5'
2	2	967	5MC	C2'-C1'-N1-C2
1	1	1962	5MC	O4'-C1'-N1-C6
2	2	966	2MG	C2'-C1'-N9-C4
1	1	2030	6MZ	O4'-C4'-C5'-O5'
2	2	966	2MG	C2'-C1'-N9-C8
1	1	746	PSU	O4'-C1'-C5-C6
1	1	2580	PSU	O4'-C1'-C5-C6
1	1	1618	6MZ	C2'-C1'-N9-C8
5	5	8	4SU	C4'-C5'-O5'-P
5	5	55	PSU	C4'-C5'-O5'-P

There are no ring outliers.

19 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	1917	PSU	1	0
1	1	1939	5MU	1	0
2	2	1407	5MC	1	0
2	2	1516	2MG	1	0
1	1	2030	6MZ	1	0
49	q	89	0TD	2	0
1	1	1835	2MG	1	0
1	1	2445	2MG	1	0
2	2	1498	UR3	1	0
2	2	516	PSU	2	0
2	2	967	5MC	1	0
2	2	966	2MG	5	0
1	1	2503	2MA	2	0
2	2	1518	MA6	2	0
2	2	1207	2MG	2	0
1	1	1915	3TD	1	0
1	1	2504	PSU	1	0
2	2	1519	MA6	3	0
1	1	1962	5MC	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 453 ligands modelled in this entry, 452 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
60	FME	5	103	5	8,9,10	0.55	0	7,9,11	1.31	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	FME	5	103	5	-	2/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	5	103	FME	O-C-CA	-3.24	116.30	124.78

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	5	103	FME	O1-CN-N-CA
60	5	103	FME	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	2196:C	O3'	2197:U	P	2.71

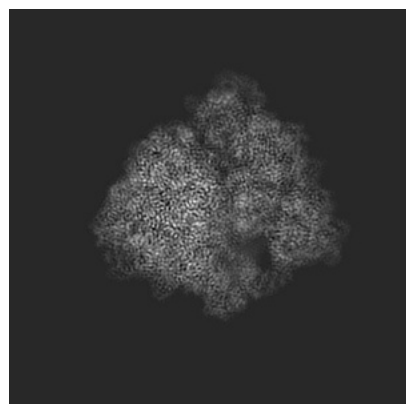
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3492. These allow visual inspection of the internal detail of the map and identification of artifacts.

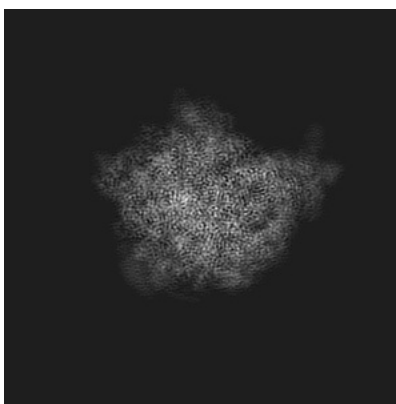
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

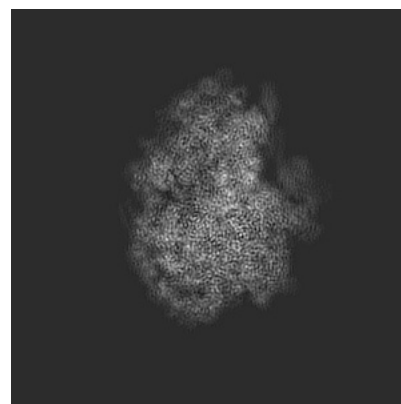
6.1.1 Primary map



X

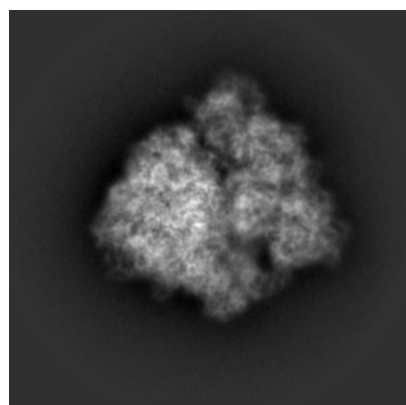


Y

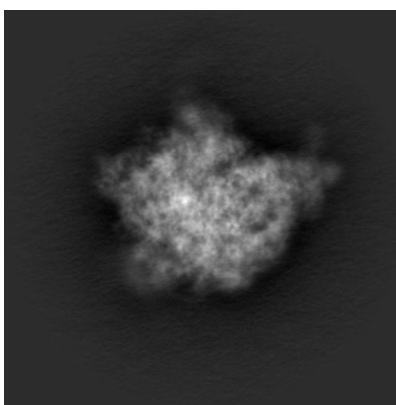


Z

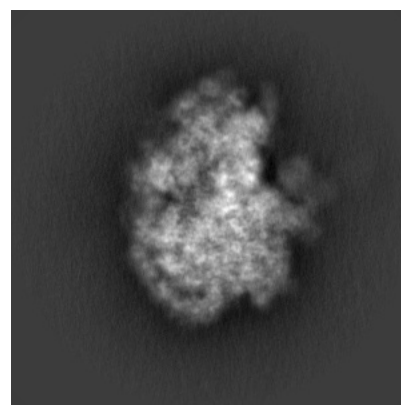
6.1.2 Raw map



X



Y

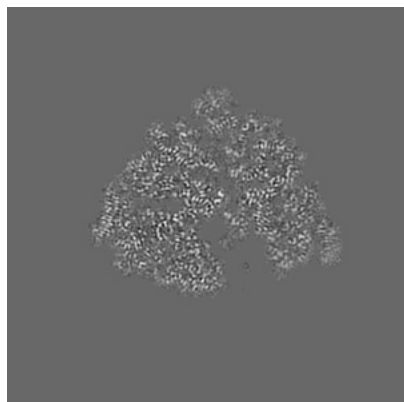


Z

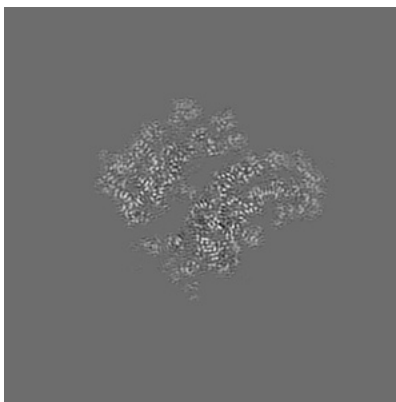
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

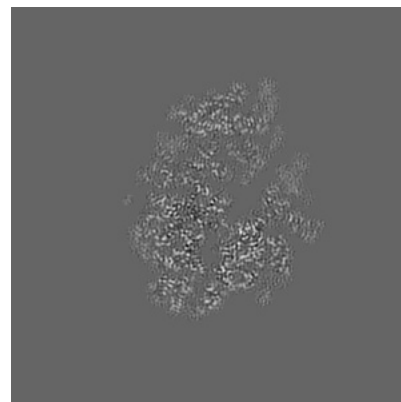
6.2.1 Primary map



X Index: 200

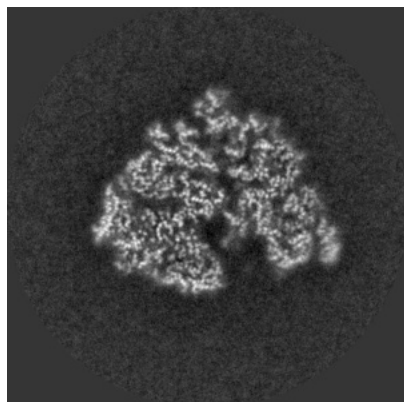


Y Index: 200

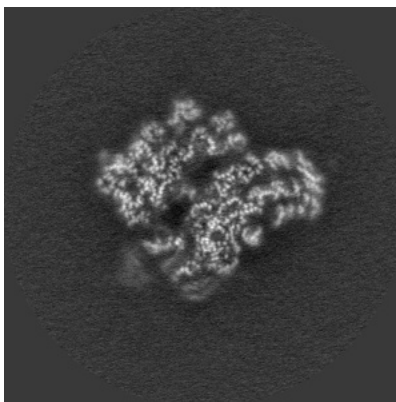


Z Index: 200

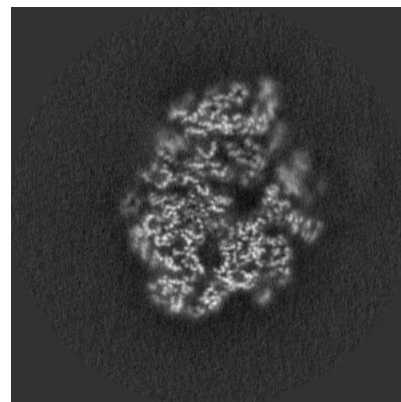
6.2.2 Raw map



X Index: 200



Y Index: 200

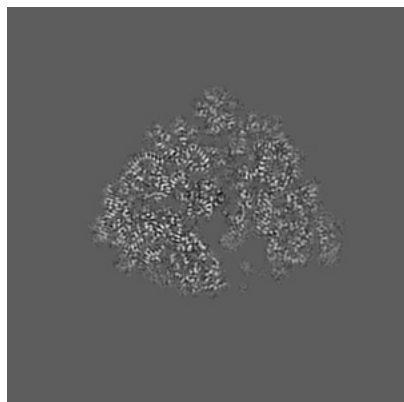


Z Index: 200

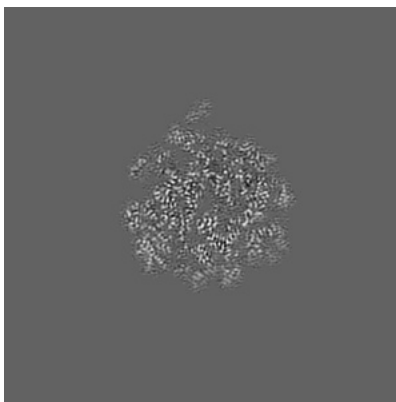
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

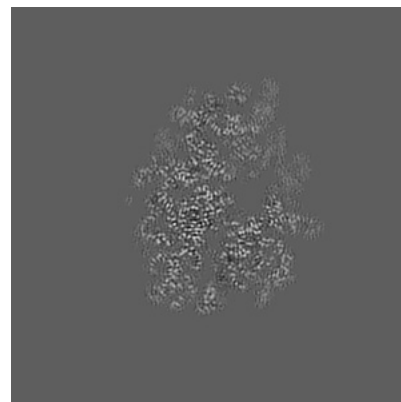
6.3.1 Primary map



X Index: 202

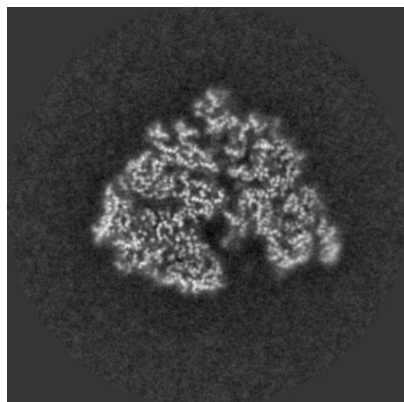


Y Index: 169

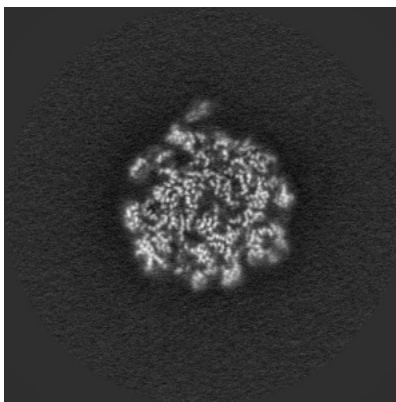


Z Index: 205

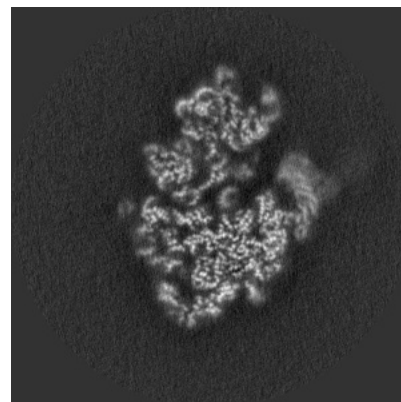
6.3.2 Raw map



X Index: 200



Y Index: 169

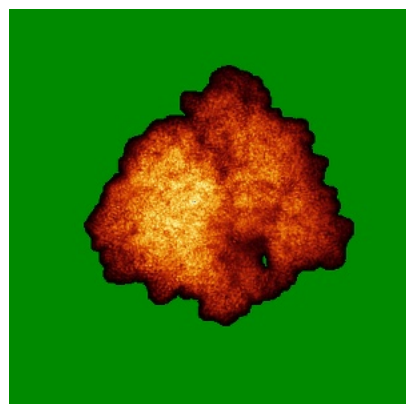


Z Index: 185

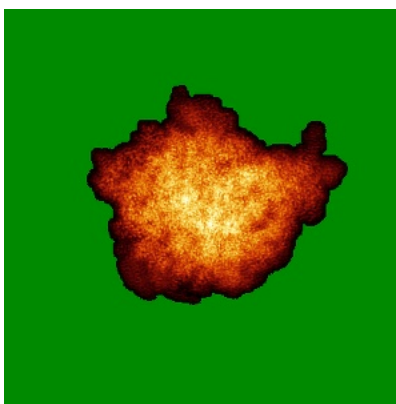
The images above show the largest variance slices of the map in three orthogonal directions.

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

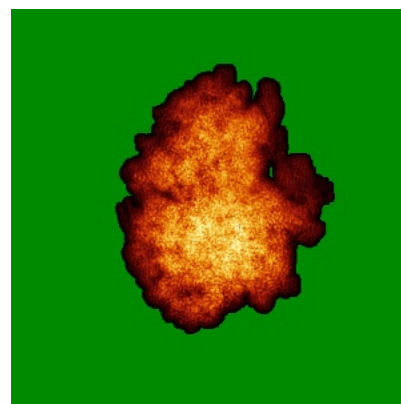
6.4.1 Primary map



X

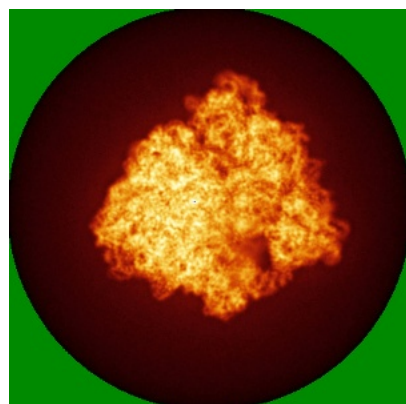


Y

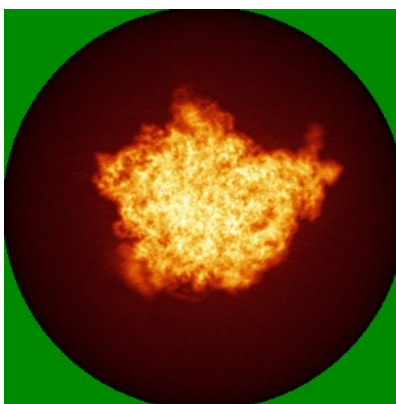


Z

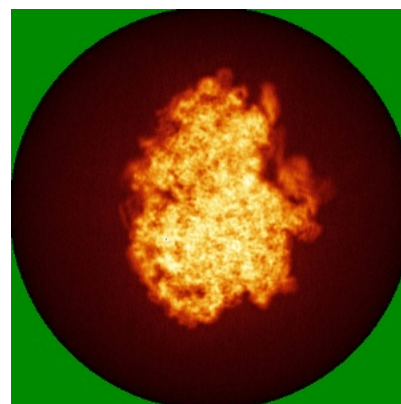
6.4.2 Raw map



X



Y



Z

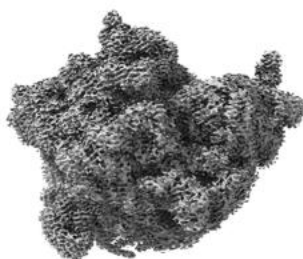
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

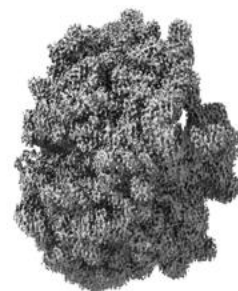
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

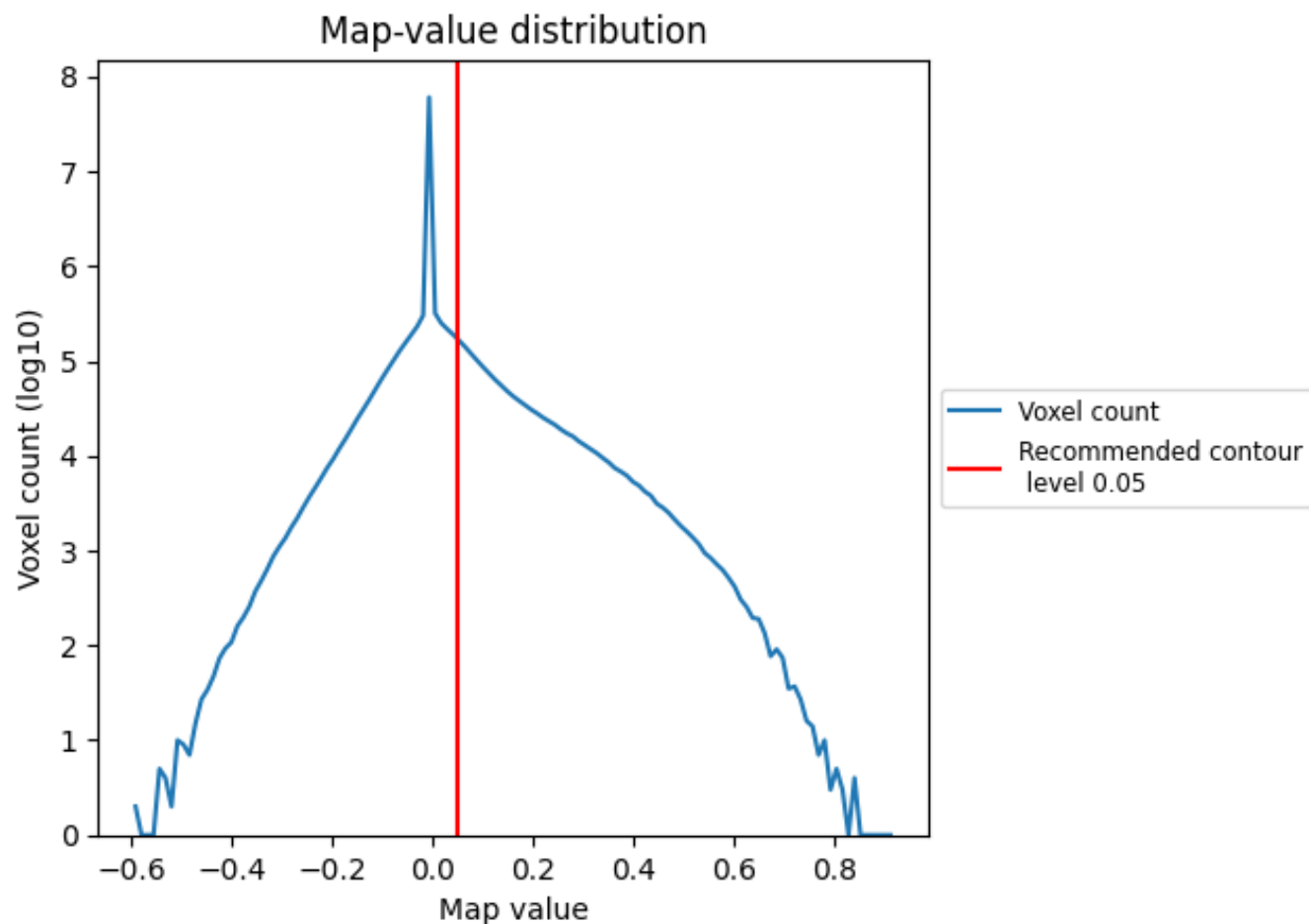
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

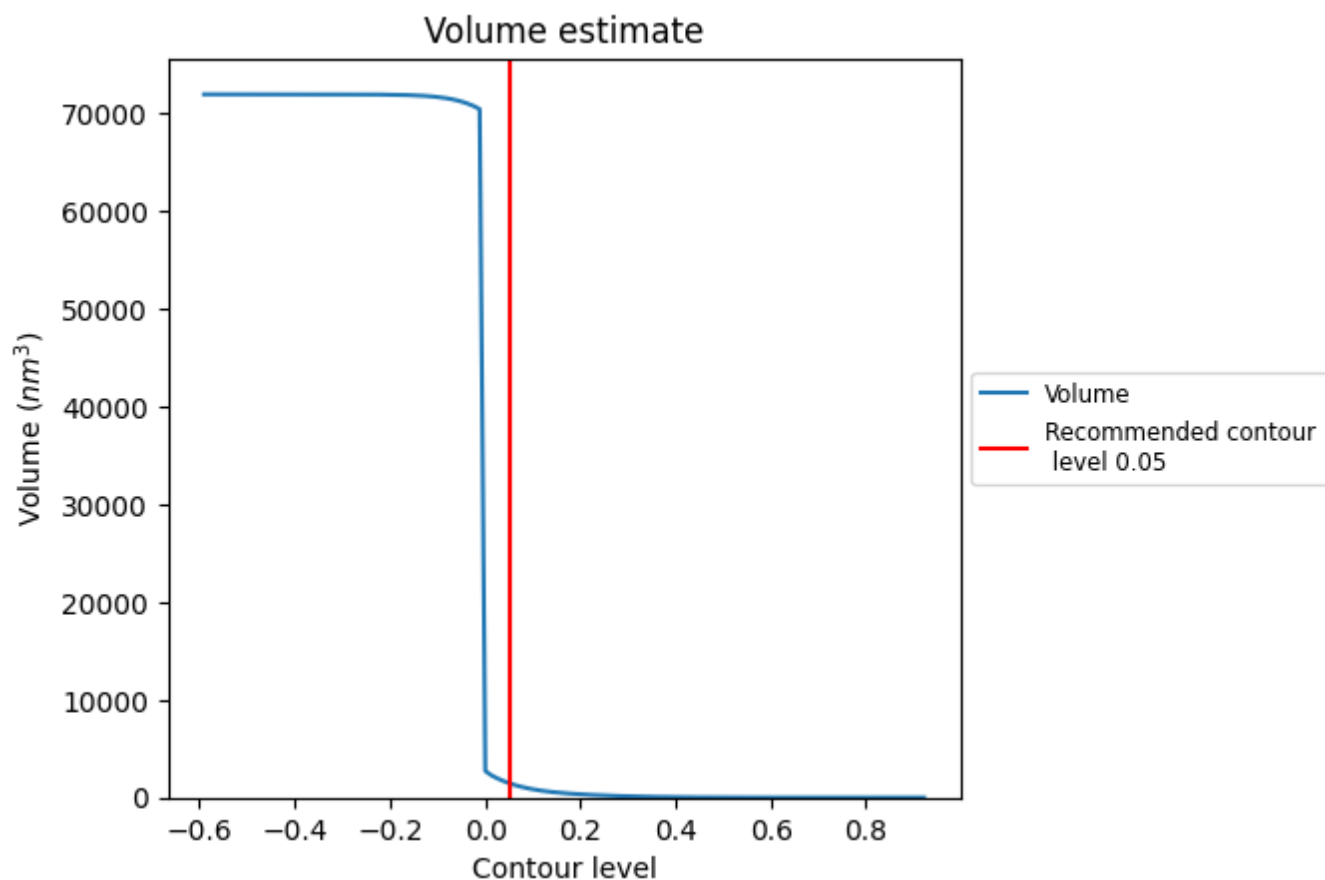
This section contains the results of statistical analysis of the map.

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.

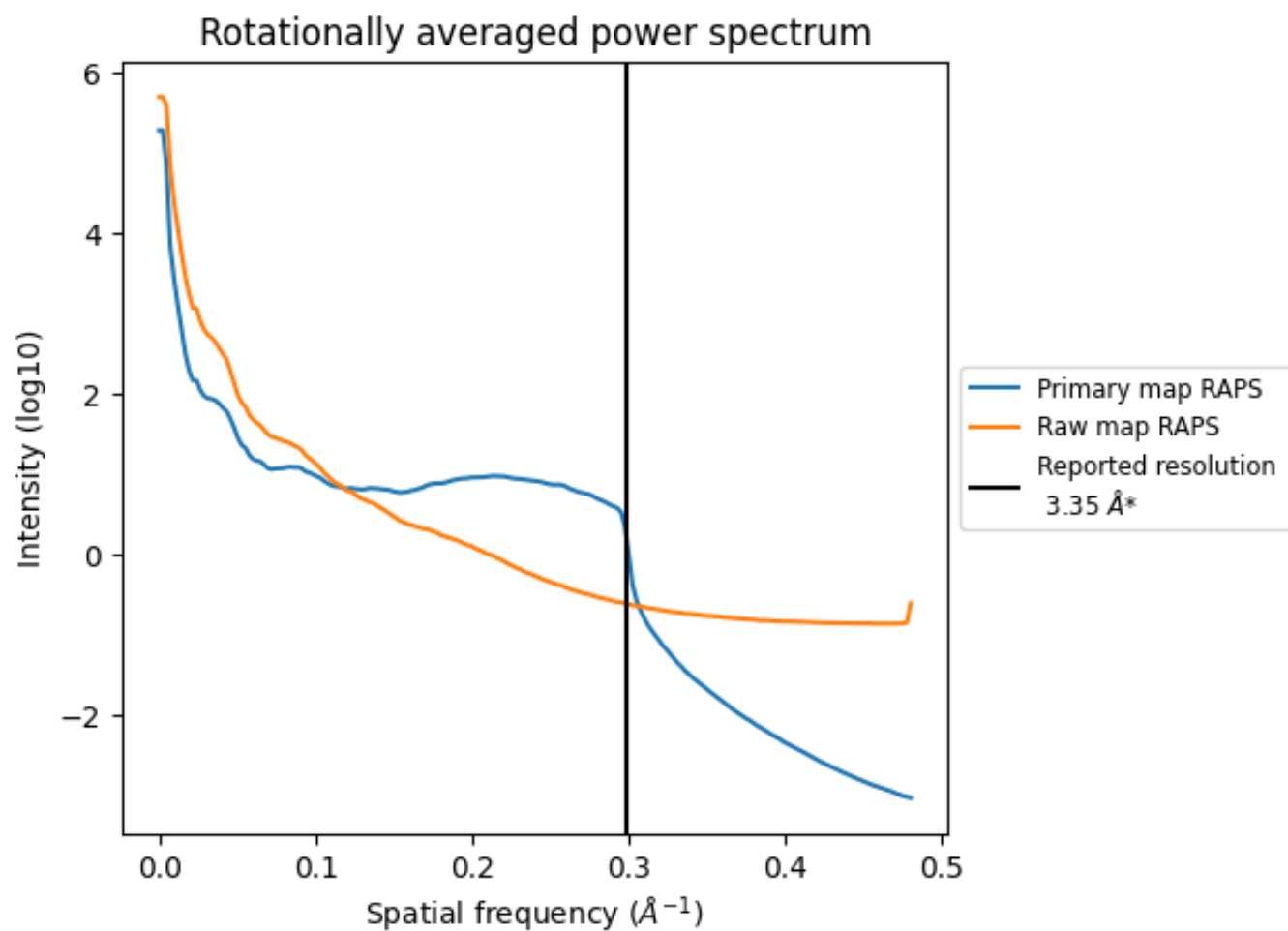
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1482 nm^3 ; this corresponds to an approximate mass of 1339 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 ⓘ

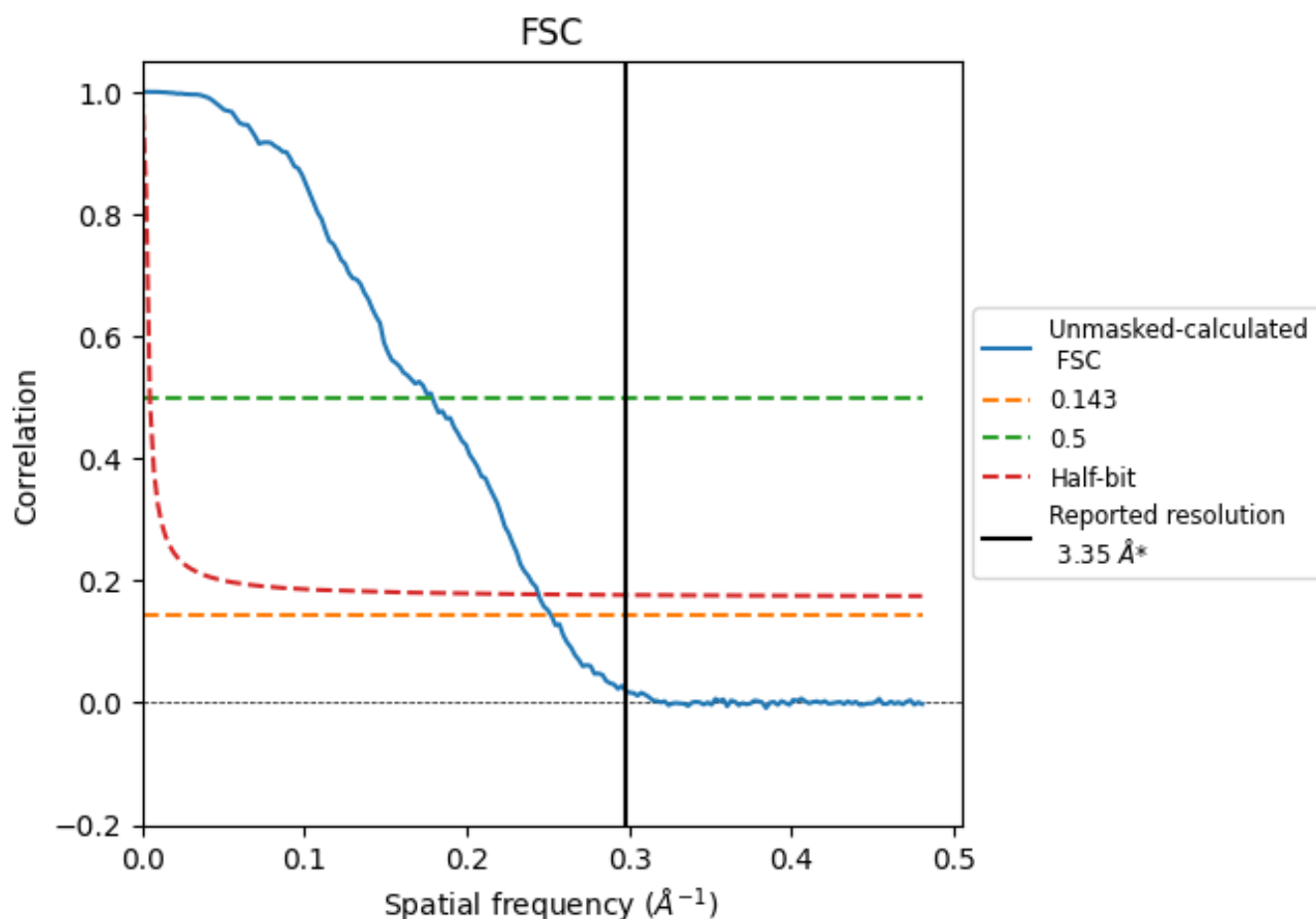


*Reported resolution corresponds to spatial frequency of $0.299 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.299 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

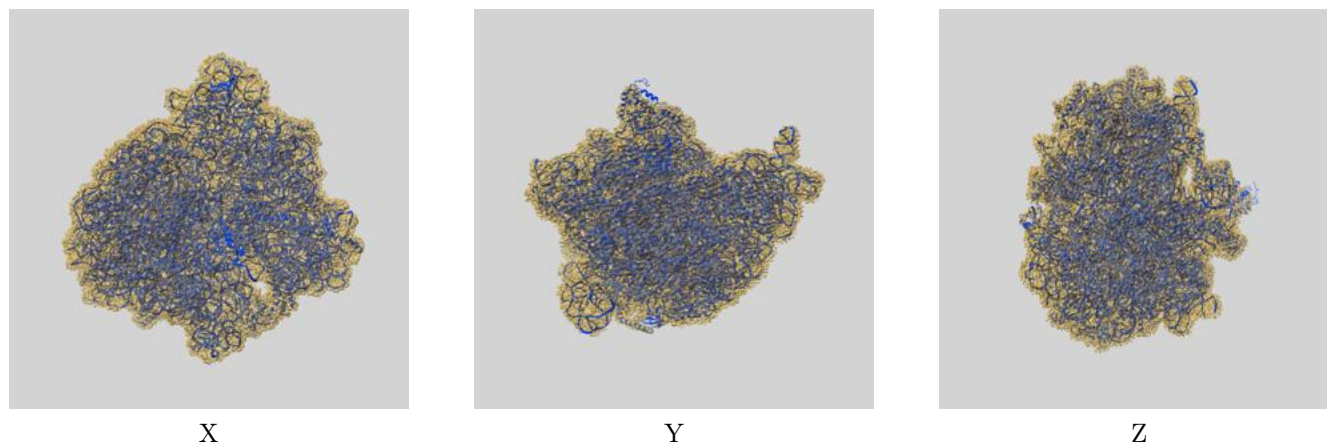
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.35	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.97	5.59	4.09

*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 3.97 differs from the reported value 3.35 by more than 10 %

9 Map-model fit [i](#)

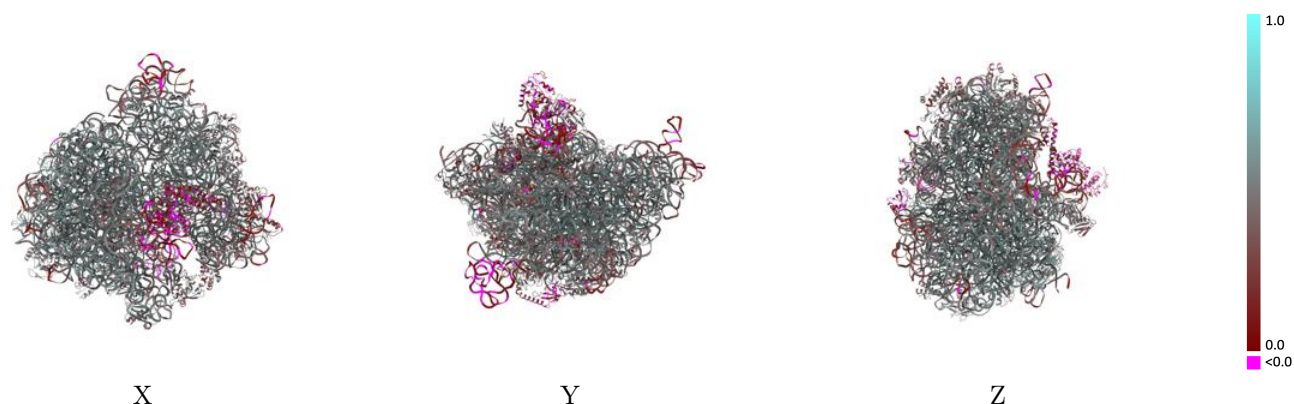
This section contains information regarding the fit between EMDB map EMD-3492 and PDB model 5MDY. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



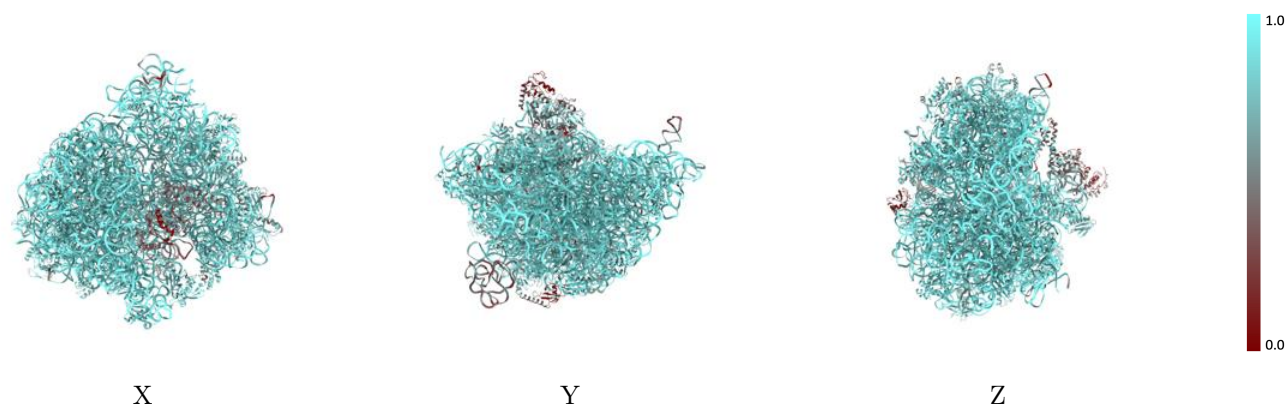
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



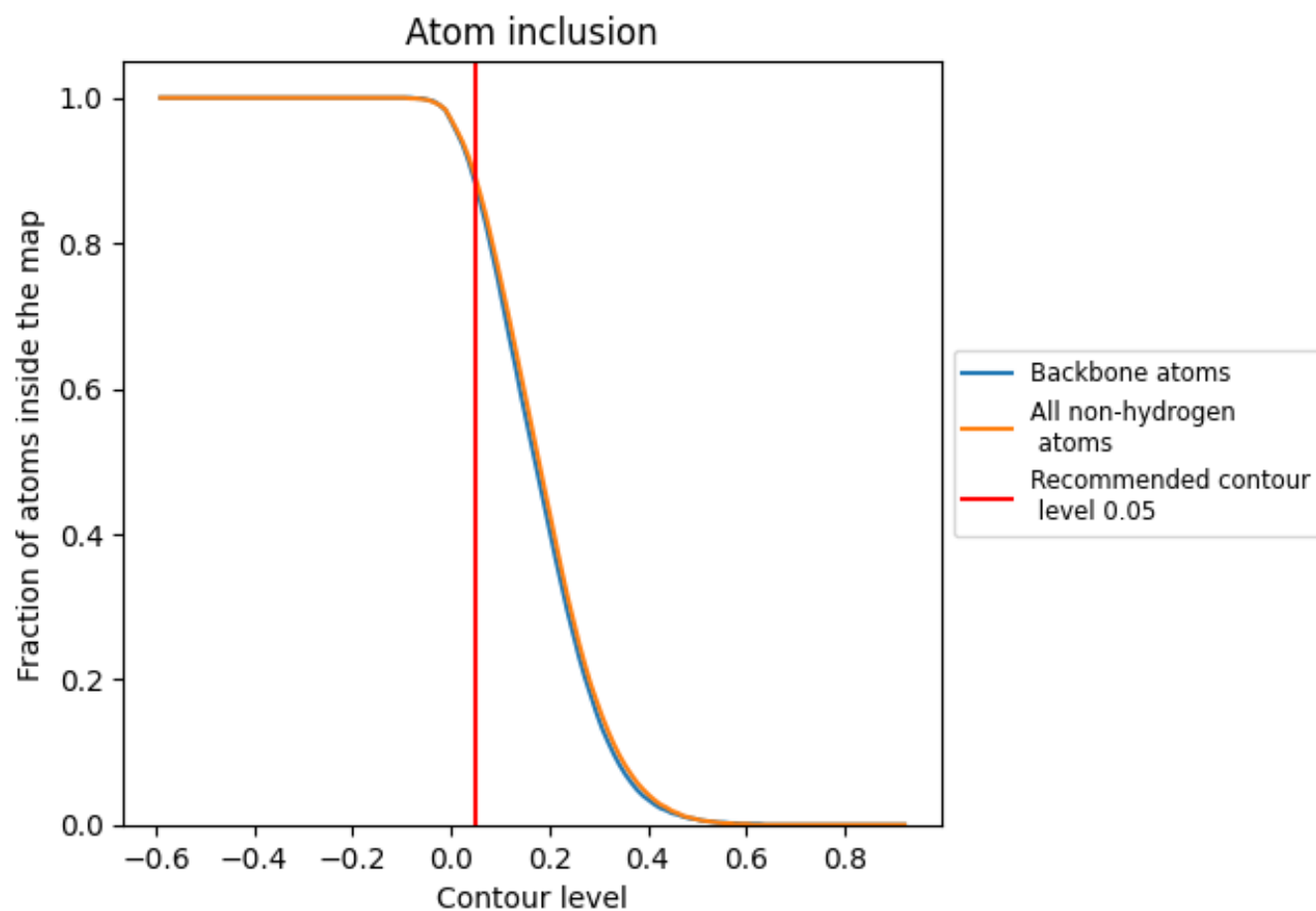
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 89% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8900	 0.4620
1	 0.9230	 0.4730
2	 0.9290	 0.4700
3	 0.9440	 0.4710
4	 0.9080	 0.4730
5	 0.8890	 0.4200
6	 0.8490	 0.4800
7	 0.6800	 0.3250
B	 0.9120	 0.5330
C	 0.9020	 0.5170
D	 0.8780	 0.4760
E	 0.8430	 0.4300
F	 0.8120	 0.4010
G	 0.4220	 0.1890
H	 0.1860	 0.0480
I	 0.4000	 0.0510
J	 0.9030	 0.5180
K	 0.8880	 0.5140
L	 0.9050	 0.5080
M	 0.9030	 0.5060
N	 0.9040	 0.5280
O	 0.8590	 0.4730
P	 0.9080	 0.5250
Q	 0.8960	 0.5180
R	 0.9220	 0.5140
S	 0.8680	 0.5130
T	 0.8590	 0.4790
U	 0.8720	 0.4560
V	 0.8520	 0.4580
W	 0.9170	 0.5510
X	 0.9130	 0.5140
Y	 0.8510	 0.4320
Z	 0.9040	 0.5210
a	 0.7980	 0.3620
b	 0.9210	 0.5230



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Chain	Atom inclusion	Q-score
c	 0.8710	 0.4980
d	 0.9210	 0.5520
e	 0.9210	 0.5480
f	 0.9180	 0.5360
g	 0.7300	 0.3670
h	 0.8490	 0.4540
i	 0.8470	 0.4510
j	 0.8880	 0.5050
k	 0.8460	 0.4390
l	 0.8070	 0.4000
m	 0.8770	 0.4970
n	 0.8600	 0.4460
o	 0.7860	 0.3960
p	 0.8540	 0.4630
q	 0.8930	 0.5070
r	 0.8530	 0.4410
s	 0.8680	 0.4580
t	 0.8480	 0.4580
u	 0.8720	 0.4790
v	 0.8720	 0.4680
w	 0.8720	 0.4770
x	 0.8660	 0.4380
y	 0.8640	 0.4750
z	 0.7780	 0.4030