



Full wwPDB EM Validation Report ⓘ

Feb 10, 2025 – 11:35 AM EST

PDB ID : 8VK0
EMDB ID : EMD-43294
Title : Structure of Mycobacterium smegmatis 50S ribosomal subunit bound to HflX:50S-HflX-A
Authors : Majumdar, S.; Koripella, R.K.; Sharma, M.R.; Manjari, S.R.; Banavali, N.K.; Agrawal, R.K.
Deposited on : 2024-01-08
Resolution : 3.14 Å (reported)
Based on initial models : 5O61, 6DZI

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:

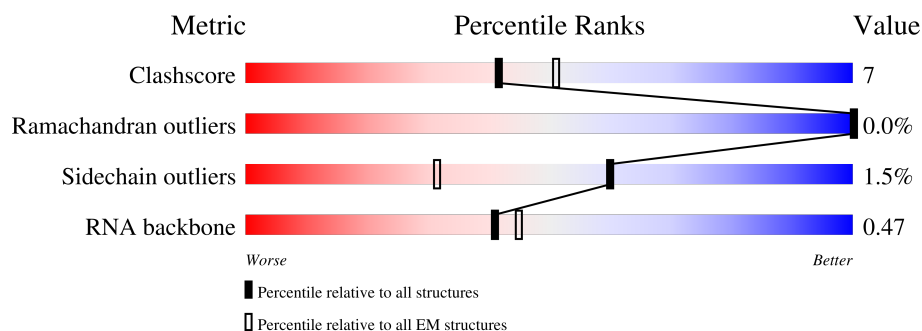
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

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 3.14 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	2	61	92% 5% .
2	3	24	83% 12% .
3	4	470	14% 24% 61% 6% 9%
4	A	3120	5% 65% 27% 7% .
5	B	118	50% 37% 9% .
6	C	278	85% 14% .
7	D	217	91% 8% .

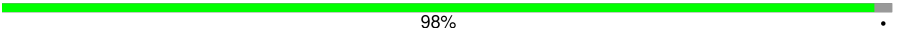
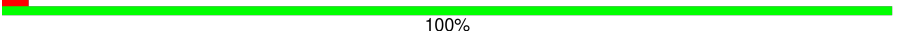

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Mol	Chain	Length	Quality of chain
8	E	215	
9	F	187	
10	G	179	
11	H	151	
12	I	175	
13	J	142	
14	K	147	
15	L	122	
16	M	147	
17	N	138	
18	O	199	
19	P	127	
20	Q	113	
21	R	129	
22	S	103	
23	T	153	
24	U	100	
25	V	105	
26	W	215	
27	X	88	
28	Y	64	
29	Z	77	
30	b	57	
31	c	55	
32	d	47	

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Mol	Chain	Length	Quality of chain
33	e	64	 98%
34	f	37	 100%
35	g	75	 41% 64% 36%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	GCP	4	501	-	-	X	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 100928 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	2	59	Total	C	N	O	0	0
			474	292	95	87		

- Molecule 2 is a protein called 50S Ribosomal Protein L37.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	3	23	Total	C	N	O	0	0
			189	111	50	28		

- Molecule 3 is a protein called GTPase HflX.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	426	Total	C	N	O	S	0	0
			3228	1997	599	625	7		

- Molecule 4 is a RNA chain called 23S ribosomal RNA.

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

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

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

- Molecule 6 is a protein called 50S ribosomal protein L2.

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

- Molecule 7 is a protein called 50S ribosomal protein L3.

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

- Molecule 8 is a protein called 50S Ribosomal Protein L4.

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

- Molecule 9 is a protein called 50S Ribosomal Protein L5.

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

- Molecule 10 is a protein called 50S ribosomal protein L6.

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

- Molecule 11 is a protein called 50S ribosomal protein L9.

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

- Molecule 12 is a protein called 50S ribosomal protein L10.

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

- Molecule 13 is a protein called 50S ribosomal protein L11.

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

- Molecule 14 is a protein called 50S Ribosomal Protein L13.

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

- Molecule 15 is a protein called 50S ribosomal protein L14.

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

- Molecule 16 is a protein called 50S ribosomal protein L15.

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

- Molecule 17 is a protein called Large ribosomal subunit protein uL16.

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

- Molecule 18 is a protein called 50S ribosomal protein L17.

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

- Molecule 19 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	126	Total	C	N	O	S	0	0
			956	586	199	171			

- Molecule 20 is a protein called 50S ribosomal protein L19.

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

- Molecule 21 is a protein called 50S Ribosomal Protein L20.

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

- Molecule 22 is a protein called 50S Ribosomal Protein L21.

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

- Molecule 23 is a protein called 50S Ribosomal Protein L22.

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

- Molecule 24 is a protein called 50S Ribosomal Protein L23.

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

- Molecule 25 is a protein called 50S ribosomal protein L24.

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

- Molecule 26 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	W	192	Total	C	N	O	0	0
			1428	881	255	292		

- Molecule 27 is a protein called 50S ribosomal protein L27.

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

- Molecule 28 is a protein called 50S Ribosomal Protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y	63	Total	C	N	O	S	0	0
			470	283	103	80	4		

- Molecule 29 is a protein called 50S ribosomal protein L29.

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

- Molecule 30 is a protein called 50S ribosomal protein L32.

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

- Molecule 31 is a protein called 50S Ribosomal Protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	49	Total	C	N	O	S	0	0
			405	248	82	71	4		

- Molecule 32 is a protein called 50S ribosomal protein L34.

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

- Molecule 33 is a protein called 50S ribosomal protein L35.

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

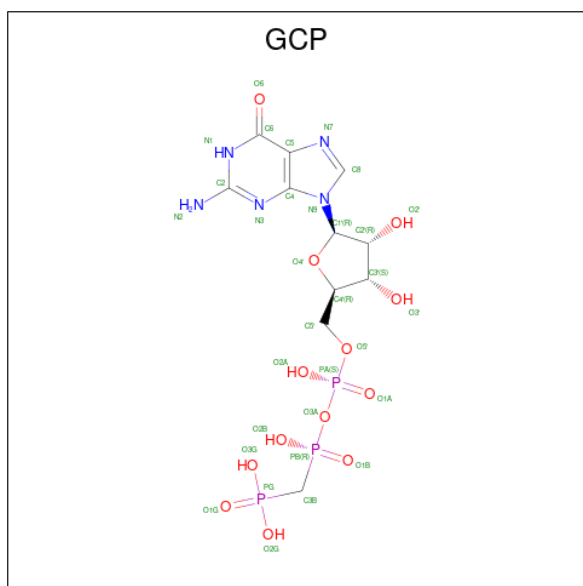
- Molecule 34 is a protein called 50S ribosomal protein L36.

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

- Molecule 35 is a protein called 50S Ribosomal Protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	48	Total	C	N	O	S	0	0
			364	225	63	71	5		

- Molecule 36 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



3 Residue-property plots


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

- Molecule 1: 50S ribosomal protein L30

Chain 2: 



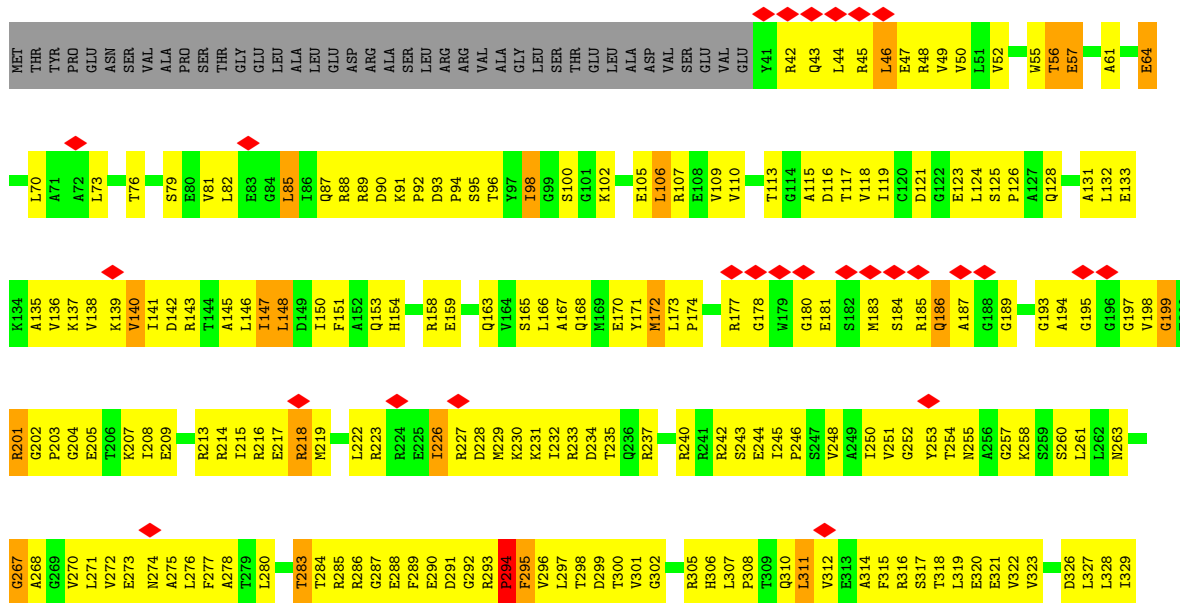
- Molecule 2: 50S Ribosomal Protein L37

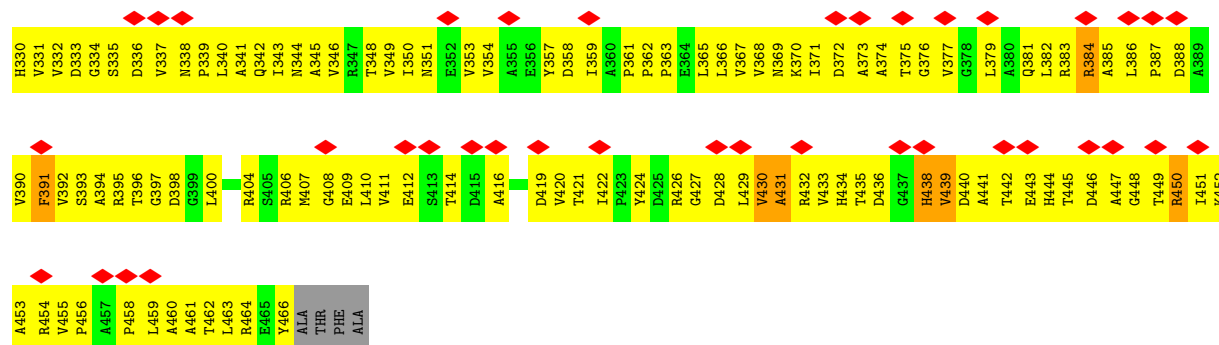
Chain 3: 



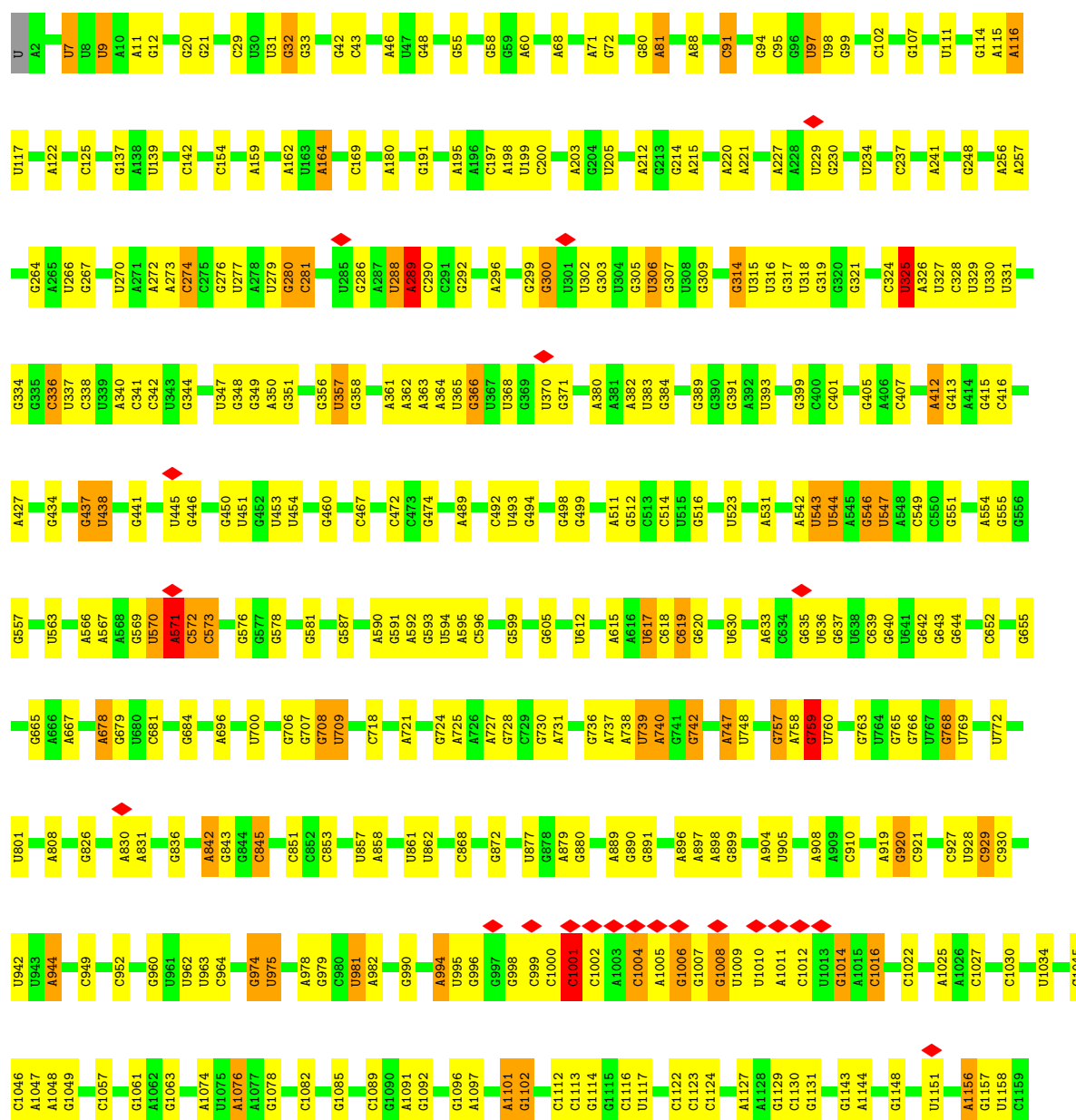
- Molecule 3: GTPase HflX

Chain 4: 

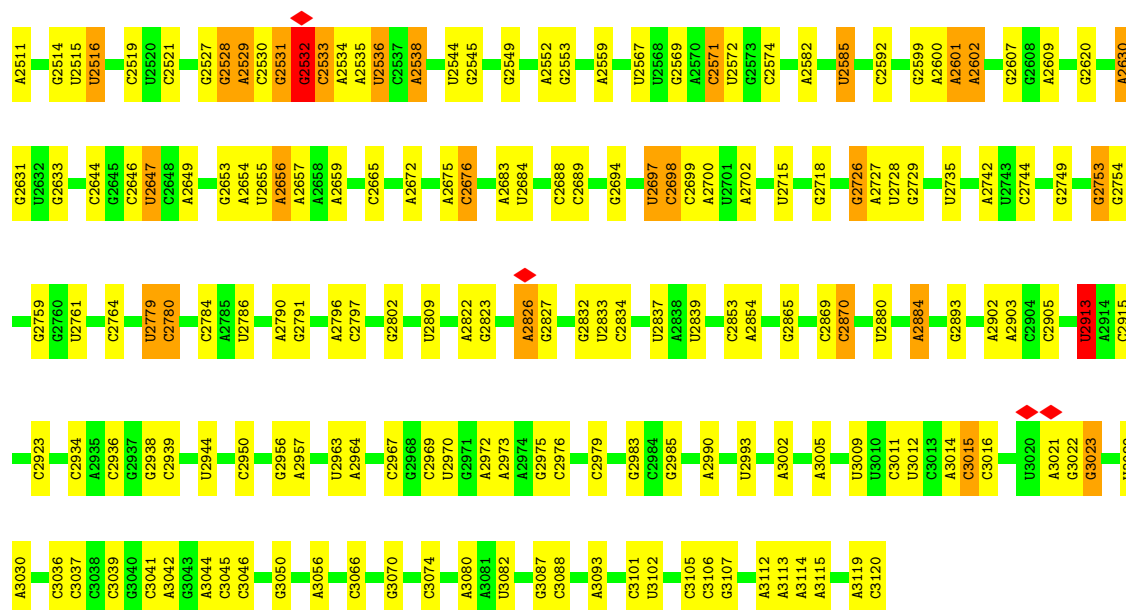




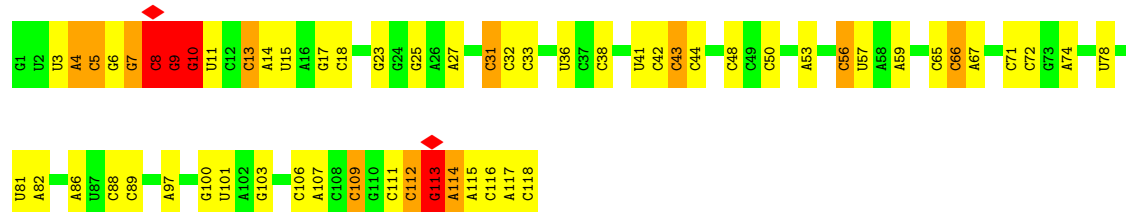
• Molecule 4: 23S ribosomal RNA



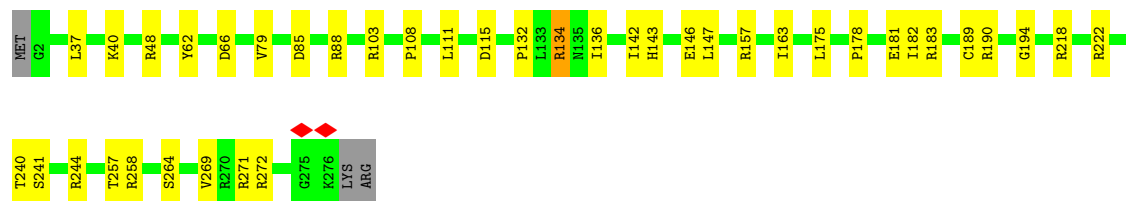
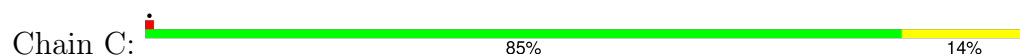
U2401	G2408	G2249	U2141	G2017	A1755	A1640	G1574	C1478	G1353	A1221	G1160
C2402	U2409	A2250	A2142	G2018	G1756	A1648	A1575	G1479	G1363	A1222	C1161
U2403	A2410	G2251	C2143	U2022	U1757	C1649	C1576	A1480	A1362	U1223	A1163
A2405	G2404	A2254	C2145	C1902	G1758	G1650	C1577	A1493	G1363	G1224	G1162
U2406	G2346	A2255	U2146	C2025	A1759	G1651	C1578	A1494	U1364	G1225	A1164
C2407	U2347	A2257	C2147	A2026	A1764	C1658	C1579	A1499	G1365	U1226	G1165
	G2408		C2148	U2033	U1767	G1669	A1580	A1499	U1371	C1227	A1166
U2409	A2349	G2260	A2151	G2034	U1767	G1670	C1581	A1508	G1377	A1228	C1170
A2410	G2413	G2263	A2152	U2035	C1768	U1671	C1582	U1509	A1377	G1230	C1171
U2411	G2414		G2153	C1912	G1769	G1672	U1583	A1510	A1380	U1231	A1172
U2412	C2352	C2267	G2154	A1916	U1777	G1673	U1584	C1513	G1381	G1232	G1173
G2413	U2353	G2268	U2155	C2043	A1778	G1674	U1585	C1513	U1382	U1234	G1174
G2414		A2045		U2044	U1778	U1675	C1586	A1518		U1235	A1175
U2418	U2354	A2046		G2045	G1786	G1677	C1587		G1386	G1237	G1176
A2421	U2355	A2070	A2161	A1931	A1787	U1678	G1588	C1521	A1387	U1237	G1177
A2422	G2356	A2071	U2163	U1939	G1788	A1679	U1589	G1522	U1388	G1238	U1178
C2423	A2357	A2071	U2164	A1940	A1789	A1680	G1590		U1389	C1239	
	A2358	G2075	C2165	A1941	U1798	U1681	G1591	G1530		G1240	U1179
C2430	G2359	A2076	A2176	G1942		G1688	U1591	C1531	G1398	G1180	G1180
C2431	C2360	C2077		G1943	G1802	U1689	G1592	G1532	A1246	G1181	
A2434	U2361	A2083	U2179	C1944	A1803	A1690	U1593	U1533	G1400	A1247	
U2435	C2362	A2084	U2180	U1945	A1803	A1691	G1594	C1534	A1401	U1248	
	A2363	C2085	U2187	U1946	C1813		G1595	C1534	A1402	G1249	U1184
C2438	C2364	U2086		A1948	C1816	C1694	C1596	A1536	A1403	U1250	A1185
G2446	A2365	C2089	A2190	A1949	C1817	U1697	G1597	A1537	A1251	G1252	A1186
A2449	C2366	U2090	C2191	A1955	C1825	G1703	U1598	A1538	A1252	C1253	A1187
C2455	G2367	U2091	A2194	G1961	A1326	U1704	G1600	U1540	G1254	G1254	A1188
G2462	C2368	G2093	U2195	G1972	C1835	C1705	U1601	A1542	C1260		A1191
G2463	C2369	G2094	G2196	A1973	G1840	A1706	U1602	A1546	A1261		
	A2370	G2095	C2209	A1974	A1844	G1707	G1603	G1547	C1269		G1192
C2467	G2371	G2096		A1975		U1709		C1548	C1270		C1193
U2467	U2372	G2099	U2215	C1978	U1847	A1713	G1606	G1549	G1271		C1194
A2470	G2373	G2107	G2216	A1981	A1848	U1717	U1607	U1551	C1272		A1195
A2471	U2374	G2107	U2217	U1982		C1718	C1608	A1552	G1273		C1196
G2472	G2375	G2107	C2218	C1978			C1609	C1553	A1274		C1197
U2473	G2376	A2113	U2219	U1981	G1851	A1716	C1610	C1554	G1275		G1198
G2474	U2377	C2116	A2221	A1990	A1852	C1718	A1611	U1555	G1276		U1199
G2475	G2377	C2117	C2224	C1991	G1863	U1723	G1615	A1556	U1292		G1201
G2476	U2378	G2128	C2224	U1992	U1864	A1729	A1616	C1557	G1293		A1202
G2477	G2379	G2129	A2227	G1993	C1866	U1730	C1617	C1558	C1298		A1203
	A2381	G2130	A2227	U1996		A1731	C1618	U1560	G1298		A1204
A2480	G2382	U2231	C2232	U1999	G1871	U1731	G1620	A1561	G1302		G1205
A2491	C2383	G2131	C2232	C2005	A1872	A1737	C1621	C1562	U1303		A1206
A2492	G2384	U2132	C2232	A2008	A1873	U1745	G1622	A1563	C1314		G1207
G2503	G2385	G2133	C2243	U2015	C1874	G1746	U1623	A1564	G1332		U1208
G2506	U2386	U2135	A2244	G2016	U1877	U1745	U1624	A1565	G1332		G1209
C2507	G2387	A2136	C2245	U2015	A1887	G1746	U1625	A1566	C1333		G1211
	G2388	C2137	U2246	U2015			G1625	C1567	G1337		U1212
	U2389	A2138	A2247						A1343		A1213
	G2390	U2139	C2248						G1343		A1214
	G2391	A2140							A1344		U1215
A2392	A2392										U1216
A2393	A2393										G1217
A2394	A2394										C1218
U2395	U2395										U1219
A2396	A2396										C1220
C2397	C2397										
C2398	C2398										
A2399	A2399										



• Molecule 5: 5S ribosomal RNA



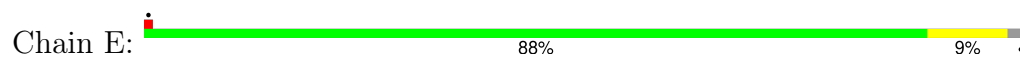
• Molecule 6: 50S ribosomal protein L2



• Molecule 7: 50S ribosomal protein L3

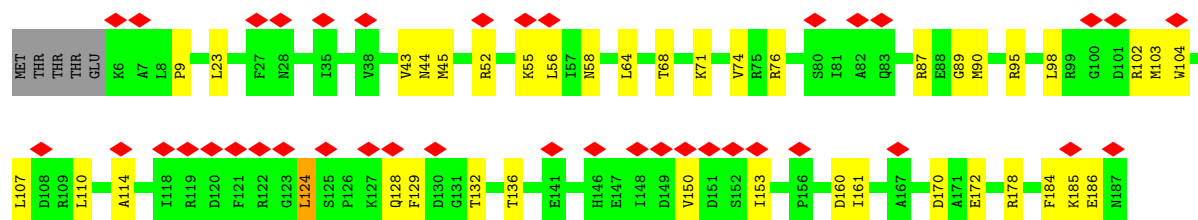
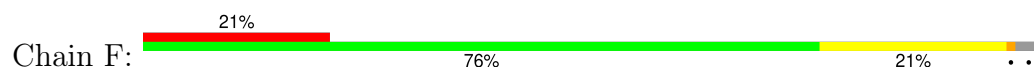


• Molecule 8: 50S Ribosomal Protein L4

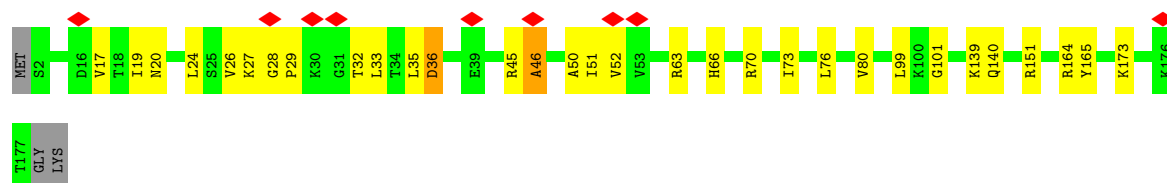
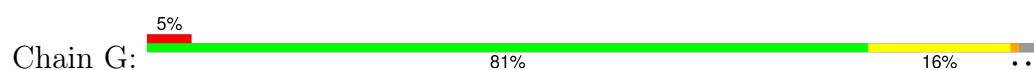




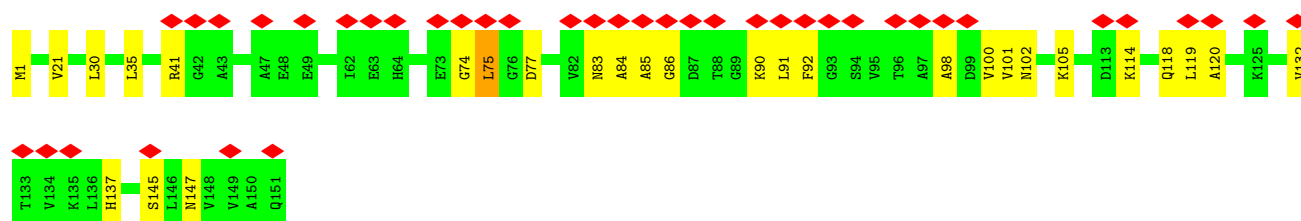
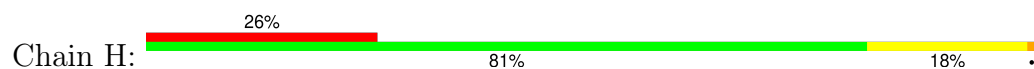
• Molecule 9: 50S Ribosomal Protein L5



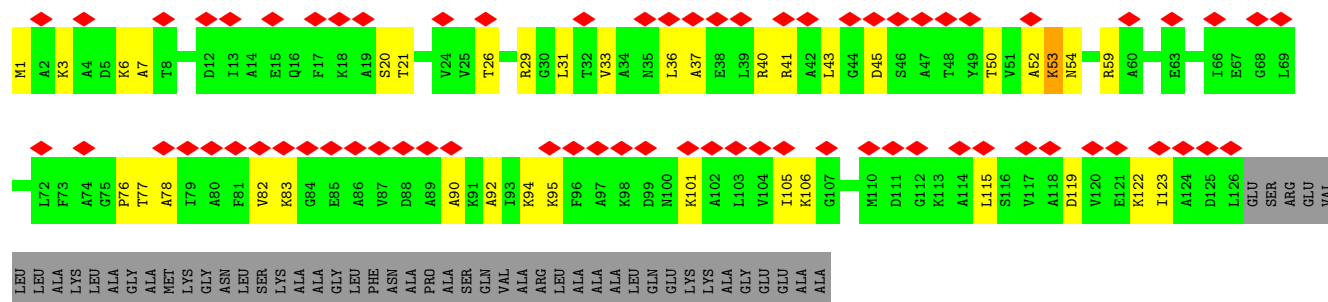
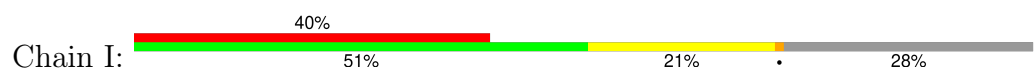
• Molecule 10: 50S ribosomal protein L6



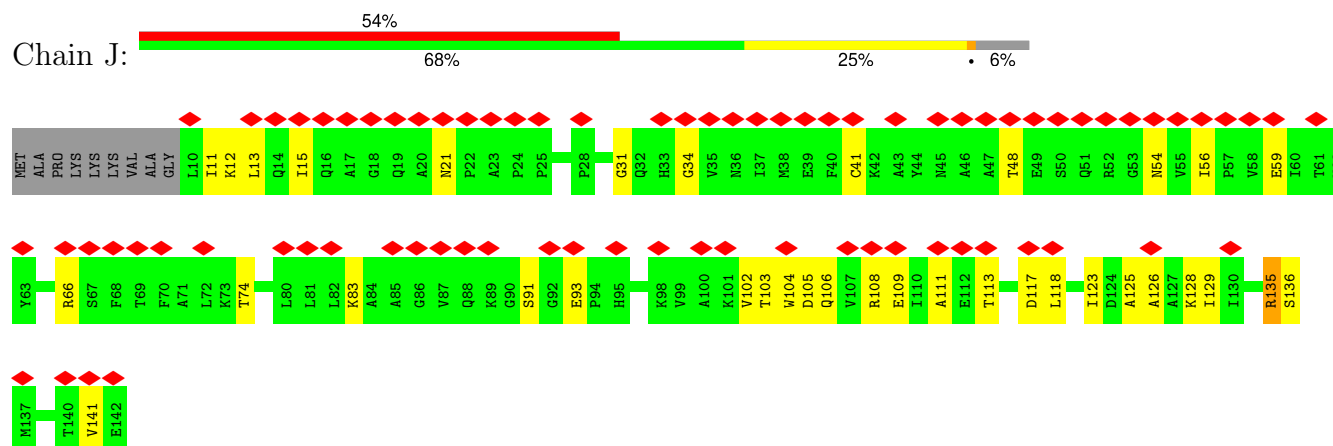
• Molecule 11: 50S ribosomal protein L9



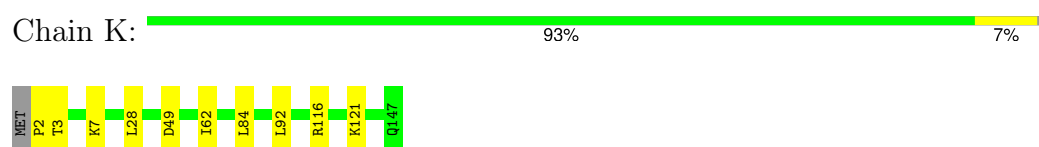
• Molecule 12: 50S ribosomal protein L10



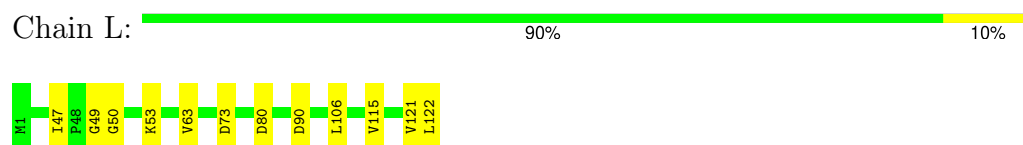
- Molecule 13: 50S ribosomal protein L11



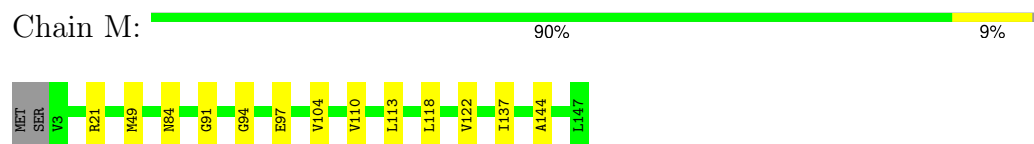
- Molecule 14: 50S Ribosomal Protein L13



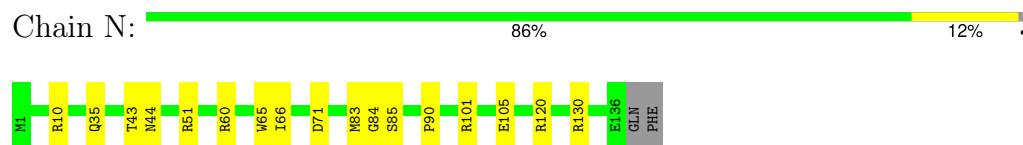
- Molecule 15: 50S ribosomal protein L14



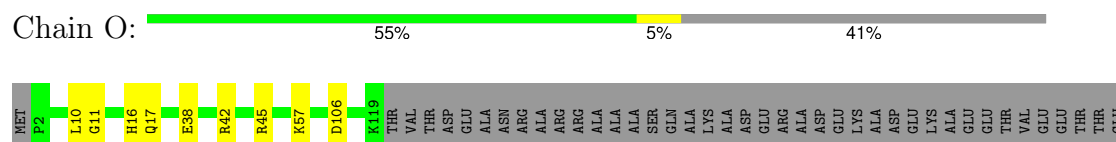
- Molecule 16: 50S ribosomal protein L15



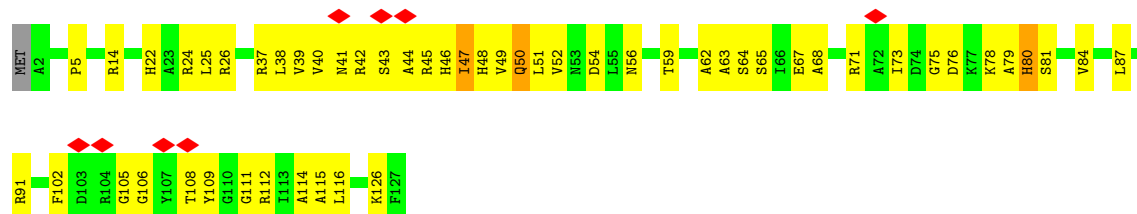
- Molecule 17: Large ribosomal subunit protein uL16



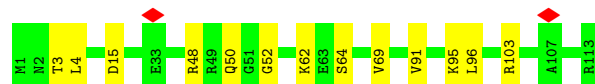
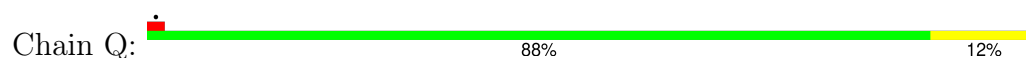
- Molecule 18: 50S ribosomal protein L17



- Molecule 19: 50S Ribosomal Protein L18



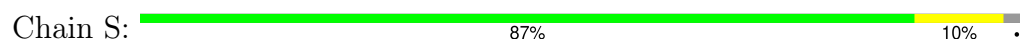
- Molecule 20: 50S ribosomal protein L19



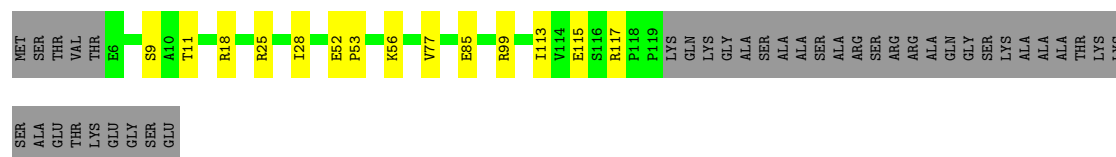
- Molecule 21: 50S Ribosomal Protein L20



- Molecule 22: 50S Ribosomal Protein L21

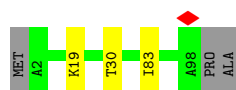


- Molecule 23: 50S Ribosomal Protein L22

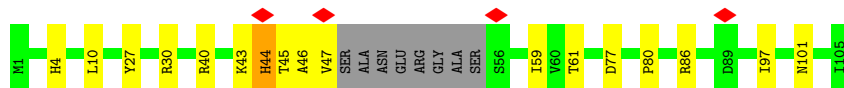
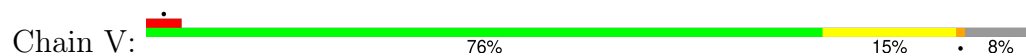


- Molecule 24: 50S Ribosomal Protein L23

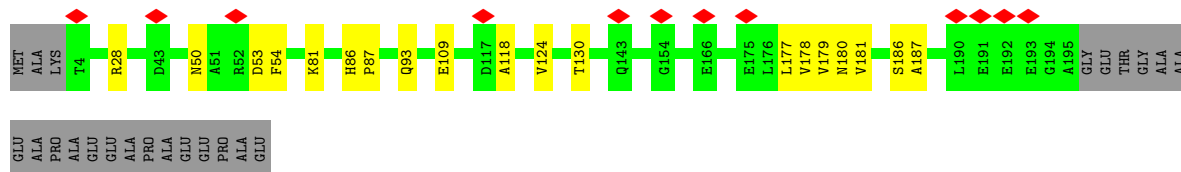
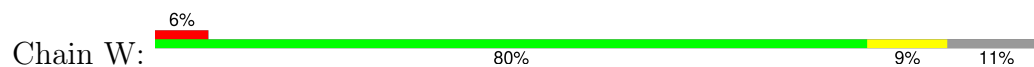




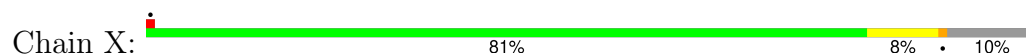
- Molecule 25: 50S ribosomal protein L24



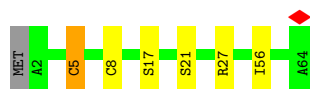
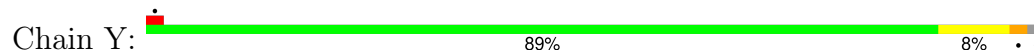
- Molecule 26: 50S ribosomal protein L25



- Molecule 27: 50S ribosomal protein L27



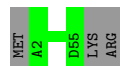
- Molecule 28: 50S Ribosomal Protein L28



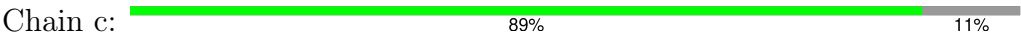
- Molecule 29: 50S ribosomal protein L29



- Molecule 30: 50S ribosomal protein L32



• Molecule 31: 50S Ribosomal Protein L33



• Molecule 32: 50S ribosomal protein L34



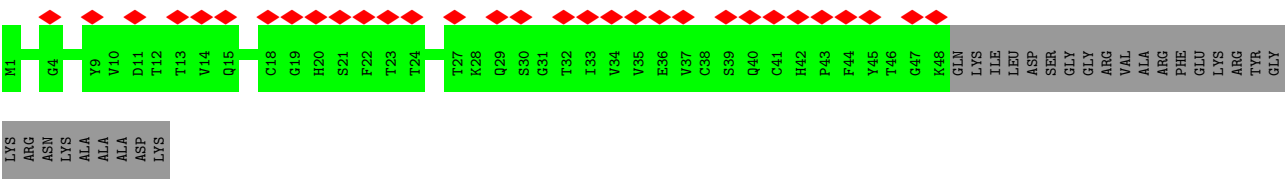
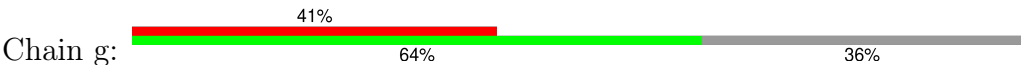
• Molecule 33: 50S ribosomal protein L35



• Molecule 34: 50S ribosomal protein L36



• Molecule 35: 50S Ribosomal Protein L31



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	57434	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 ($e^-/\text{\AA}^2$)	51.22	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.771	Depositor
Minimum map value	-0.951	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.067	Depositor
Recommended contour level	0.19	Depositor
Map size (Å)	433.19998, 433.19998, 433.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.083, 1.083, 1.083	Depositor

5 Model quality

5.1 Standard geometry

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

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	2	0.47	0/477	0.56	0/640
2	3	0.36	0/191	0.49	0/247
3	4	0.51	0/3268	0.67	3/4428 (0.1%)
4	A	0.90	1/75001 (0.0%)	1.18	566/117027 (0.5%)
5	B	0.72	0/2821	1.38	57/4396 (1.3%)
6	C	0.50	0/2153	0.58	0/2895
7	D	0.51	0/1609	0.60	0/2165
8	E	0.47	0/1592	0.61	2/2153 (0.1%)
9	F	0.32	0/1467	0.64	2/1973 (0.1%)
10	G	0.35	0/1369	0.64	0/1848
11	H	0.32	0/1027	0.68	1/1398 (0.1%)
12	I	0.31	0/925	0.64	0/1246
13	J	0.31	0/1006	0.64	0/1364
14	K	0.48	0/1157	0.54	0/1567
15	L	0.51	0/946	0.56	0/1268
16	M	0.44	0/1091	0.56	0/1457
17	N	0.43	0/1118	0.57	0/1506
18	O	0.53	0/945	0.60	0/1267
19	P	0.41	0/966	0.75	1/1298 (0.1%)
20	Q	0.49	0/921	0.62	1/1236 (0.1%)
21	R	0.54	0/1000	0.56	0/1341
22	S	0.47	0/764	0.58	0/1030
23	T	0.50	0/887	0.59	0/1204
24	U	0.50	0/766	0.56	0/1030
25	V	0.44	0/738	0.64	0/987
26	W	0.33	0/1443	0.60	0/1970
27	X	0.47	0/595	0.59	0/798
28	Y	0.47	0/478	0.55	0/641
29	Z	0.44	0/534	0.53	0/713
30	b	0.48	0/427	0.63	0/572
31	c	0.40	0/413	0.48	0/553
32	d	0.49	0/380	0.52	0/500

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	e	0.41	0/507	0.51	0/672
34	f	0.46	0/303	0.54	0/401
35	g	0.34	0/372	0.61	0/503
All	All	0.79	1/109657 (0.0%)	1.07	633/164294 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	F	0	1
10	G	0	2
11	H	0	1
12	I	0	2
13	J	0	1
18	O	0	1
19	P	0	4
26	W	0	1
All	All	0	13

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	571	A	N9-C4	6.05	1.41	1.37

All (633) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2402	C	N1-C2-O2	14.25	127.45	118.90
4	A	2402	C	N3-C2-O2	-13.03	112.78	121.90
4	A	617	U	C2-N1-C1'	11.10	131.02	117.70
4	A	1567	C	N3-C2-O2	-10.84	114.32	121.90
4	A	1220	C	C2-N1-C1'	10.53	130.38	118.80
4	A	2521	C	C6-N1-C2	-10.42	116.13	120.30
4	A	617	U	N1-C2-O2	10.38	130.07	122.80
4	A	3046	C	C2-N1-C1'	10.37	130.20	118.80
4	A	2402	C	C6-N1-C2	-10.26	116.19	120.30
4	A	1225	G	C6-C5-N7	-10.26	124.25	130.40
4	A	3046	C	N3-C2-O2	-10.19	114.76	121.90
4	A	1225	G	C4-N9-C1'	10.14	139.68	126.50
5	B	5	C	C5-C6-N1	10.06	126.03	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1608	U	C5-C6-N1	10.00	127.70	122.70
4	A	617	U	N3-C2-O2	-9.81	115.33	122.20
4	A	2025	C	N1-C2-O2	9.81	124.78	118.90
4	A	2402	C	C2-N1-C1'	9.78	129.56	118.80
4	A	2117	C	N1-C2-O2	9.64	124.68	118.90
4	A	543	U	N1-C2-O2	9.61	129.53	122.80
4	A	1225	G	N3-C4-N9	9.53	131.72	126.00
5	B	5	C	C6-N1-C2	-9.53	116.49	120.30
4	A	1534	C	N1-C2-O2	9.47	124.58	118.90
4	A	1225	G	C8-N9-C1'	-9.45	114.71	127.00
4	A	2387	U	C2-N1-C1'	9.38	128.95	117.70
4	A	1178	U	N3-C2-O2	-9.36	115.65	122.20
4	A	1567	C	N1-C2-O2	9.26	124.46	118.90
4	A	2025	C	C2-N1-C1'	9.15	128.87	118.80
4	A	1403	C	N1-C2-O2	9.09	124.35	118.90
4	A	1292	U	N3-C2-O2	-9.07	115.85	122.20
4	A	543	U	N3-C2-O2	-8.94	115.94	122.20
4	A	3046	C	C6-N1-C2	-8.94	116.72	120.30
5	B	13	C	N3-C2-O2	-8.92	115.65	121.90
4	A	1225	G	C4-C5-N7	8.89	114.36	110.80
4	A	2521	C	C2-N1-C1'	8.87	128.56	118.80
4	A	905	U	C2-N1-C1'	8.86	128.33	117.70
4	A	1403	C	N3-C2-O2	-8.81	115.73	121.90
4	A	1534	C	C2-N1-C1'	8.80	128.49	118.80
4	A	2025	C	N3-C2-O2	-8.81	115.74	121.90
4	A	1428	U	C2-N1-C1'	8.78	128.24	117.70
4	A	1224	G	N3-C2-N2	8.75	126.03	119.90
4	A	270	U	N1-C2-O2	8.71	128.90	122.80
4	A	1429	C	C2-N1-C1'	8.70	128.37	118.80
4	A	1947	U	C2-N1-C1'	8.70	128.13	117.70
4	A	1947	U	N1-C2-O2	8.69	128.88	122.80
4	A	1292	U	N1-C2-O2	8.69	128.88	122.80
4	A	1428	U	N3-C2-O2	-8.68	116.12	122.20
5	B	13	C	N1-C2-O2	8.66	124.10	118.90
5	B	32	C	C2-N1-C1'	8.64	128.31	118.80
4	A	1428	U	N1-C2-O2	8.59	128.81	122.80
4	A	2521	C	C5-C6-N1	8.54	125.27	121.00
4	A	270	U	N3-C2-O2	-8.46	116.28	122.20
5	B	13	C	C2-N1-C1'	8.46	128.11	118.80
5	B	13	C	C6-N1-C2	-8.40	116.94	120.30
4	A	2117	C	N3-C2-O2	-8.37	116.04	121.90
4	A	1638	C	C2-N1-C1'	8.36	127.99	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1947	U	N3-C2-O2	-8.35	116.36	122.20
4	A	324	C	N1-C2-O2	8.34	123.91	118.90
4	A	383	U	C2-N1-C1'	8.30	127.67	117.70
4	A	472	C	N1-C2-O2	8.29	123.88	118.90
4	A	2375	G	N3-C4-N9	8.29	130.97	126.00
4	A	2387	U	N1-C2-O2	8.28	128.60	122.80
4	A	1161	C	N3-C2-O2	-8.27	116.11	121.90
4	A	288	U	N3-C2-O2	-8.19	116.46	122.20
4	A	1225	G	N9-C4-C5	-8.19	102.13	105.40
4	A	1973	C	N3-C2-O2	-8.16	116.19	121.90
4	A	3046	C	N1-C2-O2	8.14	123.78	118.90
4	A	2402	C	C5-C6-N1	8.11	125.06	121.00
4	A	102	C	C2-N1-C1'	8.04	127.65	118.80
4	A	2944	U	N3-C2-O2	-8.03	116.58	122.20
4	A	2180	U	N1-C2-O2	8.02	128.41	122.80
4	A	1210	C	N1-C2-O2	8.02	123.71	118.90
4	A	905	U	N1-C2-O2	7.98	128.39	122.80
4	A	2387	U	N3-C2-O2	-7.97	116.62	122.20
4	A	2689	C	C2-N1-C1'	7.96	127.56	118.80
4	A	543	U	C2-N1-C1'	7.95	127.24	117.70
5	B	10	G	C8-N9-C4	-7.94	103.23	106.40
4	A	1178	U	N1-C2-O2	7.92	128.35	122.80
4	A	1403	C	C2-N1-C1'	7.89	127.48	118.80
5	B	32	C	N1-C2-O2	7.86	123.62	118.90
4	A	383	U	N3-C2-O2	-7.79	116.75	122.20
4	A	383	U	N1-C2-O2	7.79	128.25	122.80
4	A	1534	C	N3-C2-O2	-7.79	116.45	121.90
4	A	2375	G	C6-C5-N7	-7.78	125.73	130.40
4	A	1535	C	N1-C2-O2	7.74	123.54	118.90
4	A	102	C	C6-N1-C2	-7.70	117.22	120.30
4	A	472	C	C2-N1-C1'	7.66	127.23	118.80
4	A	324	C	C2-N1-C1'	7.62	127.19	118.80
4	A	1579	C	C2-N1-C1'	7.58	127.14	118.80
4	A	288	U	N1-C2-O2	7.54	128.08	122.80
4	A	619	C	C2-N1-C1'	7.53	127.08	118.80
4	A	709	U	C2-N1-C1'	7.51	126.71	117.70
4	A	1161	C	C6-N1-C2	-7.51	117.30	120.30
9	F	98	LEU	CA-CB-CG	7.47	132.49	115.30
4	A	905	U	N3-C2-O2	-7.45	116.98	122.20
4	A	617	U	C6-N1-C1'	-7.45	110.77	121.20
4	A	1694	C	C6-N1-C2	-7.41	117.34	120.30
5	B	5	C	N1-C2-O2	7.40	123.34	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	898	A	C2-N3-C4	7.35	114.28	110.60
5	B	116	C	N1-C2-O2	7.32	123.29	118.90
4	A	1220	C	C6-N1-C1'	-7.31	112.03	120.80
4	A	1597	G	N3-C4-C5	-7.29	124.95	128.60
4	A	1215	U	C2-N1-C1'	7.28	126.44	117.70
4	A	2327	C	N1-C2-O2	7.27	123.26	118.90
5	B	116	C	N3-C2-O2	-7.27	116.81	121.90
4	A	2477	G	C6-C5-N7	-7.26	126.04	130.40
4	A	962	U	C2-N1-C1'	7.25	126.39	117.70
5	B	111	C	N3-C2-O2	-7.24	116.83	121.90
4	A	9	U	N3-C2-O2	-7.24	117.13	122.20
4	A	1847	U	N3-C2-O2	-7.23	117.14	122.20
4	A	1171	C	N1-C2-O2	7.21	123.23	118.90
4	A	1161	C	N1-C2-O2	7.21	123.23	118.90
4	A	2287	C	N1-C2-O2	7.18	123.21	118.90
4	A	3011	C	C6-N1-C2	-7.18	117.43	120.30
4	A	1681	U	C2-N1-C1'	7.18	126.31	117.70
4	A	2647	U	N1-C2-O2	7.15	127.80	122.80
4	A	1567	C	C6-N1-C2	-7.14	117.44	120.30
4	A	1429	C	C6-N1-C2	-7.13	117.45	120.30
4	A	1220	C	C6-N1-C2	-7.09	117.47	120.30
4	A	1170	C	N1-C2-O2	7.05	123.13	118.90
5	B	112	C	C6-N1-C2	-7.04	117.48	120.30
4	A	2180	U	N3-C2-O2	-7.03	117.28	122.20
4	A	472	C	N3-C2-O2	-7.02	116.98	121.90
4	A	709	U	N3-C2-O2	-7.00	117.30	122.20
4	A	949	C	C6-N1-C2	-6.98	117.51	120.30
4	A	1591	U	C2-N1-C1'	6.98	126.07	117.70
4	A	571	A	C2-N3-C4	6.96	114.08	110.60
4	A	2320	C	O4'-C1'-N1	6.96	113.77	108.20
4	A	1210	C	C2-N1-C1'	6.95	126.44	118.80
4	A	2287	C	N3-C2-O2	-6.93	117.05	121.90
4	A	1421	C	C6-N1-C2	-6.92	117.53	120.30
4	A	1534	C	C6-N1-C2	-6.92	117.53	120.30
4	A	2944	U	N1-C2-O2	6.92	127.64	122.80
5	B	72	C	C2-N1-C1'	6.88	126.37	118.80
4	A	1333	C	C2-N1-C1'	6.86	126.35	118.80
4	A	2287	C	C6-N1-C2	-6.84	117.56	120.30
4	A	1239	C	C6-N1-C2	-6.83	117.57	120.30
4	A	2025	C	C6-N1-C1'	-6.82	112.62	120.80
4	A	1477	C	C5-C6-N1	6.81	124.41	121.00
4	A	974	G	P-O3'-C3'	6.81	127.87	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1123	C	C6-N1-C2	-6.80	117.58	120.30
4	A	1292	U	C2-N1-C1'	6.80	125.86	117.70
4	A	2435	U	N3-C2-O2	-6.80	117.44	122.20
19	P	38	LEU	CA-CB-CG	6.79	130.92	115.30
4	A	1224	G	N1-C2-N2	-6.78	110.10	116.20
4	A	2362	C	N1-C2-O2	6.78	122.97	118.90
4	A	619	C	N1-C2-O2	6.78	122.97	118.90
4	A	853	C	C2-N1-C1'	6.76	126.24	118.80
4	A	2321	U	C5-C6-N1	6.76	126.08	122.70
4	A	2647	U	C2-N1-C1'	6.75	125.79	117.70
4	A	1429	C	C5-C6-N1	6.74	124.37	121.00
4	A	9	U	C2-N1-C1'	6.73	125.78	117.70
4	A	1597	G	C4-N9-C1'	6.71	135.23	126.50
5	B	32	C	C6-N1-C2	-6.70	117.62	120.30
4	A	1045	C	C2-N1-C1'	6.70	126.17	118.80
4	A	169	C	C2-N1-C1'	6.70	126.17	118.80
4	A	324	C	C5-C6-N1	6.69	124.34	121.00
4	A	700	U	N3-C2-O2	-6.68	117.53	122.20
5	B	31	C	C2-N1-C1'	6.68	126.15	118.80
4	A	1421	C	C5-C6-N1	6.67	124.34	121.00
4	A	1260	C	C2-N1-C1'	6.67	126.13	118.80
3	4	199	GLY	N-CA-C	-6.66	96.44	113.10
4	A	1210	C	N3-C2-O2	-6.66	117.24	121.90
4	A	2880	U	N1-C2-O2	6.66	127.47	122.80
4	A	2321	U	O5'-P-OP1	-6.66	99.70	105.70
4	A	740	A	O4'-C1'-N9	6.66	113.53	108.20
4	A	102	C	C5-C6-N1	6.64	124.32	121.00
4	A	929	C	C5-C6-N1	6.64	124.32	121.00
5	B	10	G	O4'-C1'-N9	6.64	113.51	108.20
4	A	1535	C	N3-C2-O2	-6.64	117.25	121.90
4	A	2780	C	C6-N1-C2	-6.63	117.65	120.30
4	A	2993	U	N3-C2-O2	-6.63	117.56	122.20
4	A	1597	G	N3-C4-N9	6.63	129.98	126.00
4	A	324	C	C6-N1-C2	-6.62	117.65	120.30
4	A	1681	U	N1-C2-O2	6.61	127.43	122.80
4	A	2375	G	C4-N9-C1'	6.61	135.09	126.50
4	A	2870	C	C6-N1-C2	-6.61	117.66	120.30
4	A	2521	C	N1-C2-O2	6.60	122.86	118.90
4	A	274	C	C2-N1-C1'	6.60	126.06	118.80
4	A	1220	C	C5-C6-N1	6.60	124.30	121.00
4	A	2398	C	C6-N1-C2	-6.57	117.67	120.30
4	A	1587	G	N3-C4-C5	-6.57	125.31	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1441	C	N1-C2-O2	6.57	122.84	118.90
4	A	1535	C	C6-N1-C2	-6.55	117.68	120.30
4	A	1694	C	C2-N1-C1'	6.54	125.99	118.80
4	A	2325	U	N3-C2-O2	-6.54	117.62	122.20
4	A	929	C	C6-N1-C2	-6.53	117.69	120.30
4	A	2005	C	C6-N1-C2	-6.53	117.69	120.30
4	A	709	U	N1-C2-O2	6.52	127.36	122.80
4	A	2267	C	C6-N1-C2	-6.52	117.69	120.30
4	A	1638	C	N1-C2-O2	6.51	122.81	118.90
4	A	2296	C	C6-N1-C2	-6.51	117.70	120.30
4	A	2375	G	N9-C4-C5	-6.51	102.80	105.40
4	A	2327	C	N3-C2-O2	-6.50	117.35	121.90
4	A	1429	C	N1-C2-O2	6.48	122.79	118.90
4	A	2870	C	C5-C6-N1	6.48	124.24	121.00
4	A	2697	U	O4'-C1'-N1	6.47	113.38	108.20
4	A	1694	C	C5-C6-N1	6.46	124.23	121.00
4	A	3011	C	C5-C6-N1	6.46	124.23	121.00
5	B	6	G	N3-C4-N9	6.45	129.87	126.00
4	A	547	U	N1-C2-O2	6.44	127.31	122.80
4	A	325	U	N3-C2-O2	-6.44	117.69	122.20
5	B	32	C	N3-C2-O2	-6.44	117.39	121.90
4	A	3046	C	C6-N1-C1'	-6.44	113.07	120.80
4	A	325	U	C2-N1-C1'	6.43	125.42	117.70
4	A	1220	C	N1-C2-O2	6.43	122.76	118.90
4	A	2375	G	C8-N9-C1'	-6.42	118.65	127.00
4	A	29	C	C2-N1-C1'	6.41	125.85	118.80
4	A	2345	U	P-O3'-C3'	6.40	127.38	119.70
4	A	1239	C	C5-C6-N1	6.39	124.20	121.00
4	A	191	G	C4-N9-C1'	6.38	134.79	126.50
4	A	325	U	N1-C2-O2	6.36	127.25	122.80
4	A	1260	C	C6-N1-C2	-6.35	117.76	120.30
4	A	3036	C	N1-C2-O2	6.34	122.71	118.90
4	A	619	C	N3-C2-O2	-6.34	117.46	121.90
4	A	1102	G	N3-C4-C5	-6.33	125.44	128.60
4	A	111	U	C2-N1-C1'	6.32	125.29	117.70
4	A	1587	G	C4-N9-C1'	6.30	134.69	126.50
4	A	2232	C	C6-N1-C2	-6.29	117.78	120.30
5	B	31	C	N1-C2-O2	6.28	122.67	118.90
4	A	1567	C	C2-N1-C1'	6.26	125.69	118.80
4	A	277	U	N3-C2-O2	-6.26	117.82	122.20
5	B	7	G	N3-C4-N9	-6.25	122.25	126.00
4	A	1061	G	C4-N9-C1'	6.25	134.62	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1535	C	C2-N1-C1'	6.24	125.67	118.80
4	A	2477	G	N1-C2-N3	6.24	127.65	123.90
4	A	270	U	C2-N1-C1'	6.24	125.19	117.70
4	A	324	C	N3-C2-O2	-6.24	117.53	121.90
4	A	2005	C	C5-C6-N1	6.23	124.12	121.00
4	A	2430	C	C2-N1-C1'	6.21	125.64	118.80
11	H	75	LEU	CA-CB-CG	6.21	129.59	115.30
4	A	3011	C	C2-N1-C1'	6.20	125.62	118.80
4	A	1206	A	OP2-P-O3'	6.18	118.79	105.20
4	A	2477	G	N7-C8-N9	6.18	116.19	113.10
4	A	2880	U	N3-C2-O2	-6.17	117.88	122.20
4	A	197	C	C5-C6-N1	6.17	124.08	121.00
4	A	1617	C	C6-N1-C2	-6.17	117.83	120.30
4	A	288	U	C5-C6-N1	6.16	125.78	122.70
5	B	6	G	C4-N9-C1'	6.16	134.51	126.50
4	A	102	C	N1-C2-O2	6.16	122.59	118.90
4	A	2698	C	N1-C2-O2	6.16	122.59	118.90
4	A	1006	G	N1-C6-O6	-6.14	116.22	119.90
4	A	1448	C	C6-N1-C2	-6.13	117.85	120.30
4	A	2375	G	C4-C5-N7	6.12	113.25	110.80
4	A	2689	C	C6-N1-C2	-6.12	117.85	120.30
4	A	2647	U	N3-C2-O2	-6.12	117.92	122.20
4	A	1225	G	N7-C8-N9	6.11	116.16	113.10
4	A	2295	C	C5-C6-N1	6.11	124.05	121.00
4	A	1638	C	C5-C6-N1	6.10	124.05	121.00
4	A	2779	U	P-O3'-C3'	6.10	127.03	119.70
4	A	2387	U	C6-N1-C1'	-6.10	112.66	121.20
4	A	2699	C	C6-N1-C2	-6.10	117.86	120.30
4	A	1276	G	N3-C4-N9	6.10	129.66	126.00
5	B	88	C	C2-N1-C1'	6.09	125.50	118.80
4	A	2327	C	C6-N1-C2	-6.08	117.87	120.30
4	A	288	U	C6-N1-C2	-6.07	117.36	121.00
4	A	1903	C	C2-N1-C1'	6.07	125.47	118.80
4	A	962	U	N3-C2-O2	-6.05	117.96	122.20
4	A	277	U	N1-C2-O2	6.05	127.04	122.80
4	A	2684	U	N3-C2-O2	-6.05	117.97	122.20
4	A	1681	U	N3-C2-O2	-6.04	117.97	122.20
4	A	2366	C	N3-C2-O2	-6.04	117.67	121.90
4	A	1183	U	C2-N1-C1'	6.04	124.95	117.70
4	A	1276	G	C4-N9-C1'	6.04	134.35	126.50
4	A	2409	U	C2-N1-C1'	6.04	124.94	117.70
5	B	31	C	C6-N1-C2	-6.04	117.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1638	C	C6-N1-C2	-6.03	117.89	120.30
4	A	1171	C	N3-C2-O2	-6.03	117.68	121.90
4	A	454	U	C2-N1-C1'	6.02	124.92	117.70
4	A	2698	C	C2-N1-C1'	6.02	125.42	118.80
4	A	1403	C	C6-N1-C2	-6.01	117.90	120.30
4	A	962	U	N1-C2-O2	6.00	127.00	122.80
4	A	1973	C	C6-N1-C1'	6.00	128.00	120.80
4	A	289	A	C2-N3-C4	6.00	113.60	110.60
4	A	1947	U	P-O3'-C3'	5.97	126.87	119.70
4	A	1531	C	C5-C6-N1	5.97	123.99	121.00
4	A	2477	G	C4-N9-C1'	5.97	134.26	126.50
4	A	2689	C	C5-C6-N1	5.97	123.99	121.00
4	A	999	C	N3-C2-O2	-5.96	117.72	121.90
4	A	1225	G	N3-C2-N2	5.96	124.08	119.90
4	A	964	C	C6-N1-C2	-5.96	117.92	120.30
4	A	1230	G	C5-C6-O6	5.96	132.17	128.60
4	A	2086	U	C2-N1-C1'	5.95	124.84	117.70
4	A	2075	G	O4'-C1'-N9	5.95	112.96	108.20
4	A	1817	C	C5-C6-N1	5.95	123.97	121.00
4	A	1651	C	C6-N1-C2	-5.95	117.92	120.30
4	A	759	G	N3-C4-C5	5.94	131.57	128.60
4	A	845	C	C6-N1-C2	-5.94	117.92	120.30
4	A	2780	C	C5-C6-N1	5.94	123.97	121.00
4	A	2335	G	N3-C4-C5	-5.94	125.63	128.60
4	A	2335	G	N3-C4-N9	5.94	129.56	126.00
4	A	2993	U	N1-C2-O2	5.92	126.95	122.80
4	A	1172	A	O4'-C1'-N9	5.92	112.94	108.20
4	A	1477	C	C6-N1-C2	-5.92	117.93	120.30
4	A	1165	G	C8-N9-C4	-5.92	104.03	106.40
4	A	1170	C	C5-C6-N1	5.92	123.96	121.00
4	A	1123	C	C5-C6-N1	5.91	123.96	121.00
4	A	191	G	C8-N9-C1'	-5.91	119.32	127.00
4	A	630	U	N3-C2-O2	-5.91	118.06	122.20
5	B	6	G	C8-N9-C1'	-5.91	119.32	127.00
4	A	2780	C	N1-C2-O2	5.90	122.44	118.90
4	A	2571	C	C2-N1-C1'	5.89	125.28	118.80
4	A	571	A	N3-C4-C5	-5.89	122.67	126.80
4	A	1978	C	N1-C2-O2	5.89	122.44	118.90
4	A	1816	C	C2-N1-C1'	5.89	125.28	118.80
4	A	1817	C	C6-N1-C2	-5.88	117.95	120.30
4	A	1123	C	C2-N1-C1'	5.88	125.27	118.80
4	A	357	U	P-O3'-C3'	5.88	126.75	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1030	C	C2-N1-C1'	5.88	125.27	118.80
4	A	2430	C	C6-N1-C2	-5.88	117.95	120.30
5	B	72	C	N1-C2-O2	5.88	122.43	118.90
4	A	1082	C	C5-C6-N1	5.87	123.93	121.00
4	A	1448	C	C5-C6-N1	5.87	123.94	121.00
4	A	2243	C	C2-N1-C1'	5.87	125.26	118.80
4	A	2455	C	C6-N1-C2	-5.87	117.95	120.30
4	A	1458	G	C4-N9-C1'	5.86	134.12	126.50
4	A	2688	C	C5-C6-N1	5.86	123.93	121.00
5	B	8	C	C5-C6-N1	5.86	123.93	121.00
4	A	407	C	C6-N1-C2	-5.86	117.96	120.30
4	A	2477	G	N1-C2-N2	-5.85	110.93	116.20
4	A	1608	U	C6-N1-C2	-5.85	117.49	121.00
4	A	1816	C	C6-N1-C2	-5.84	117.96	120.30
5	B	10	G	N7-C8-N9	5.84	116.02	113.10
4	A	29	C	C5-C6-N1	5.84	123.92	121.00
4	A	2077	C	C6-N1-C2	-5.84	117.97	120.30
5	B	72	C	C5-C6-N1	5.84	123.92	121.00
4	A	905	U	C6-N1-C1'	-5.83	113.03	121.20
4	A	599	G	O4'-C1'-N9	5.83	112.86	108.20
4	A	1767	U	C5-C6-N1	5.83	125.61	122.70
4	A	472	C	C6-N1-C2	-5.83	117.97	120.30
4	A	234	U	N3-C2-O2	-5.82	118.12	122.20
4	A	1597	G	C2-N3-C4	5.82	114.81	111.90
4	A	205	U	N1-C2-O2	5.81	126.86	122.80
4	A	547	U	C2-N1-C1'	5.81	124.67	117.70
4	A	1678	U	C2-N1-C1'	5.80	124.66	117.70
4	A	1816	C	C5-C6-N1	5.80	123.90	121.00
4	A	205	U	N3-C2-O2	-5.79	118.15	122.20
4	A	139	U	C2-N1-C1'	5.79	124.64	117.70
4	A	3015	C	C2-N1-C1'	5.79	125.16	118.80
4	A	1276	G	C8-N9-C1'	-5.78	119.48	127.00
4	A	1333	C	C5-C6-N1	5.78	123.89	121.00
4	A	2086	U	N1-C2-O2	5.78	126.85	122.80
4	A	9	U	N1-C2-O2	5.78	126.84	122.80
4	A	237	C	N1-C2-O2	5.78	122.37	118.90
4	A	336	C	P-O3'-C3'	5.75	126.61	119.70
3	4	294	PRO	N-CA-C	5.75	127.06	112.10
5	B	5	C	C2-N3-C4	5.75	122.77	119.90
5	B	56	C	C6-N1-C2	-5.74	118.00	120.30
4	A	1991	C	C6-N1-C2	-5.73	118.01	120.30
4	A	2423	C	C6-N1-C2	-5.73	118.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	32	C	C6-N1-C1'	-5.73	113.93	120.80
4	A	2295	C	C6-N1-C2	-5.73	118.01	120.30
4	A	2934	C	C6-N1-C2	-5.72	118.01	120.30
4	A	2085	C	C2-N1-C1'	5.72	125.09	118.80
4	A	2409	U	N1-C2-O2	5.72	126.80	122.80
5	B	114	A	O4'-C1'-N9	5.72	112.78	108.20
4	A	1467	U	N3-C2-O2	-5.71	118.20	122.20
4	A	2230	C	C5-C6-N1	5.71	123.86	121.00
5	B	7	G	N3-C4-C5	5.71	131.46	128.60
4	A	1428	U	C6-N1-C1'	-5.71	113.21	121.20
4	A	1638	C	C6-N1-C1'	-5.70	113.96	120.80
4	A	2521	C	N3-C2-O2	-5.70	117.91	121.90
5	B	18	C	C2-N1-C1'	5.70	125.07	118.80
4	A	1045	C	N3-C2-O2	-5.70	117.91	121.90
4	A	1531	C	C6-N1-C2	-5.69	118.02	120.30
4	A	1579	C	C5-C6-N1	5.69	123.84	121.00
4	A	2287	C	C2-N1-C1'	5.69	125.06	118.80
4	A	2979	C	N1-C2-O2	5.69	122.31	118.90
4	A	1224	G	N9-C4-C5	-5.68	103.13	105.40
4	A	1534	C	C6-N1-C1'	-5.68	113.98	120.80
4	A	2913	U	N3-C2-O2	-5.67	118.23	122.20
4	A	630	U	N1-C2-O2	5.67	126.77	122.80
4	A	2322	C	C6-N1-C2	-5.67	118.03	120.30
4	A	3037	C	C6-N1-C2	-5.67	118.03	120.30
4	A	438	U	N3-C2-O2	-5.67	118.23	122.20
4	A	2325	U	N1-C2-O2	5.67	126.77	122.80
4	A	1549	G	O4'-C1'-N9	5.66	112.73	108.20
4	A	547	U	N3-C2-O2	-5.65	118.24	122.20
4	A	454	U	C5-C6-N1	5.65	125.53	122.70
5	B	5	C	C2-N1-C1'	5.65	125.02	118.80
4	A	91	C	C2-N1-C1'	5.65	125.01	118.80
4	A	974	G	OP2-P-O3'	5.65	117.62	105.20
4	A	1996	U	C2-N1-C1'	5.64	124.47	117.70
4	A	1061	G	C8-N9-C1'	-5.64	119.66	127.00
4	A	1597	G	C8-N9-C1'	-5.64	119.67	127.00
4	A	2117	C	C2-N1-C1'	5.63	125.00	118.80
4	A	2979	C	C2-N1-C1'	5.63	124.99	118.80
4	A	1429	C	C6-N1-C1'	-5.62	114.06	120.80
4	A	2409	U	N3-C2-O2	-5.62	118.27	122.20
4	A	514	C	C6-N1-C2	-5.61	118.06	120.30
4	A	1610	C	C2-N1-C1'	5.61	124.97	118.80
5	B	65	C	C2-N1-C1'	5.61	124.97	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	274	C	C6-N1-C2	-5.60	118.06	120.30
4	A	1183	U	N3-C2-O2	-5.60	118.28	122.20
4	A	2366	C	N1-C2-O2	5.60	122.26	118.90
5	B	72	C	C6-N1-C2	-5.59	118.06	120.30
4	A	975	U	C2-N1-C1'	5.59	124.41	117.70
4	A	2975	G	N1-C6-O6	-5.59	116.55	119.90
4	A	1874	C	C6-N1-C2	-5.58	118.07	120.30
4	A	2698	C	N3-C2-O2	-5.57	118.00	121.90
4	A	2684	U	N1-C2-O2	5.57	126.70	122.80
4	A	2869	C	C2-N1-C1'	5.57	124.92	118.80
4	A	97	U	P-O3'-C3'	5.56	126.37	119.70
4	A	681	C	C5-C6-N1	5.56	123.78	121.00
4	A	277	U	C2-N1-C1'	5.56	124.37	117.70
4	A	1292	U	P-O3'-C3'	5.56	126.37	119.70
4	A	3045	C	C6-N1-C2	-5.54	118.08	120.30
4	A	1579	C	N1-C2-O2	5.54	122.22	118.90
4	A	191	G	O4'-C1'-N9	5.54	112.63	108.20
4	A	1214	A	O4'-C1'-N9	5.54	112.63	108.20
4	A	1333	C	N1-C2-O2	5.53	122.22	118.90
4	A	237	C	C2-N1-C1'	5.53	124.88	118.80
4	A	1224	G	C8-N9-C1'	-5.53	119.82	127.00
4	A	2402	C	C6-N1-C1'	-5.52	114.17	120.80
4	A	1386	G	C8-N9-C4	-5.52	104.19	106.40
4	A	2532	G	C4-N9-C1'	5.52	133.67	126.50
5	B	9	G	C5-N7-C8	-5.51	101.54	104.30
4	A	3036	C	N3-C2-O2	-5.50	118.05	121.90
4	A	2689	C	N1-C2-O2	5.50	122.20	118.90
4	A	288	U	C2-N1-C1'	5.50	124.29	117.70
4	A	2656	A	P-O3'-C3'	5.49	126.29	119.70
4	A	1082	C	C6-N1-C2	-5.49	118.11	120.30
4	A	1170	C	C6-N1-C2	-5.49	118.11	120.30
4	A	2467	U	N3-C2-O2	-5.49	118.36	122.20
4	A	571	A	N3-C4-N9	5.48	131.79	127.40
4	A	1587	G	N3-C4-N9	5.48	129.29	126.00
4	A	1610	C	N1-C2-O2	5.48	122.19	118.90
5	B	8	C	C6-N1-C2	-5.48	118.11	120.30
4	A	29	C	N1-C2-O2	5.47	122.18	118.90
4	A	1182	C	C5-C6-N1	5.47	123.73	121.00
4	A	43	C	C2-N1-C1'	5.47	124.81	118.80
5	B	32	C	C5-C6-N1	5.47	123.73	121.00
4	A	1260	C	N3-C2-O2	-5.46	118.08	121.90
5	B	111	C	C6-N1-C2	-5.46	118.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	842	A	P-O3'-C3'	5.46	126.26	119.70
5	B	66	C	N1-C2-O2	5.46	122.18	118.90
4	A	1554	U	N3-C2-O2	-5.46	118.38	122.20
4	A	1204	A	C4-N9-C1'	5.46	136.12	126.30
4	A	1235	U	OP2-P-O3'	5.46	117.20	105.20
4	A	2165	C	N1-C2-O2	5.45	122.17	118.90
4	A	2438	C	N1-C2-O2	5.45	122.17	118.90
4	A	2688	C	C2-N1-C1'	5.45	124.80	118.80
4	A	169	C	C6-N1-C2	-5.45	118.12	120.30
4	A	1571	C	C2-N1-C1'	5.44	124.79	118.80
4	A	1230	G	P-O3'-C3'	5.43	126.22	119.70
4	A	549	C	C6-N1-C2	-5.42	118.13	120.30
4	A	2269	C	C6-N1-C2	-5.42	118.13	120.30
4	A	2944	U	C2-N1-C1'	5.42	124.20	117.70
4	A	930	C	C6-N1-C2	-5.41	118.14	120.30
8	E	148	LEU	CA-CB-CG	5.41	127.75	115.30
4	A	1117	U	N3-C2-O2	-5.41	118.42	122.20
4	A	1993	G	C4-N9-C1'	5.41	133.53	126.50
4	A	2435	U	C2-N1-C1'	5.40	124.19	117.70
4	A	2155	U	C2-N1-C1'	5.40	124.18	117.70
4	A	1183	U	N1-C2-O2	5.40	126.58	122.80
4	A	1901	C	C5-C6-N1	5.40	123.70	121.00
4	A	1947	U	C6-N1-C1'	-5.40	113.64	121.20
4	A	1171	C	C6-N1-C2	-5.40	118.14	120.30
4	A	1927	C	C2-N1-C1'	5.40	124.74	118.80
5	B	113	G	O4'-C1'-N9	5.40	112.52	108.20
4	A	981	U	P-O3'-C3'	5.39	126.17	119.70
4	A	1276	G	C6-C5-N7	-5.39	127.17	130.40
4	A	237	C	C6-N1-C2	-5.38	118.15	120.30
4	A	617	U	C5-C6-N1	5.38	125.39	122.70
4	A	1554	U	N1-C2-O2	5.38	126.57	122.80
5	B	116	C	C6-N1-C2	-5.38	118.15	120.30
5	B	56	C	N3-C2-O2	-5.37	118.14	121.90
4	A	2209	C	C5-C6-N1	5.37	123.69	121.00
4	A	199	U	N3-C2-O2	-5.36	118.45	122.20
4	A	3036	C	C6-N1-C2	-5.36	118.16	120.30
4	A	921	C	C6-N1-C2	-5.36	118.16	120.30
4	A	2375	G	C5-C6-O6	-5.36	125.39	128.60
4	A	1909	C	C6-N1-C2	-5.35	118.16	120.30
4	A	2320	C	P-O3'-C3'	5.34	126.11	119.70
4	A	199	U	N1-C2-O2	5.34	126.54	122.80
4	A	2418	U	N1-C2-O2	5.34	126.54	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1458	G	C8-N9-C1'	-5.34	120.06	127.00
4	A	963	U	N3-C2-O2	-5.33	118.47	122.20
4	A	1697	U	N3-C2-O2	-5.33	118.47	122.20
4	A	2117	C	C6-N1-C2	-5.33	118.17	120.30
4	A	619	C	C6-N1-C1'	-5.33	114.40	120.80
4	A	383	U	C6-N1-C1'	-5.33	113.74	121.20
4	A	2644	C	C6-N1-C2	-5.33	118.17	120.30
4	A	1292	U	C6-N1-C2	-5.32	117.81	121.00
4	A	2688	C	C6-N1-C2	-5.32	118.17	120.30
4	A	237	C	C5-C6-N1	5.31	123.66	121.00
4	A	2869	C	N3-C2-O2	-5.31	118.18	121.90
5	B	31	C	C5-C6-N1	5.31	123.65	121.00
9	F	124	LEU	CA-CB-CG	5.31	127.50	115.30
4	A	1124	C	C6-N1-C2	-5.30	118.18	120.30
4	A	1509	U	C6-N1-C1'	5.30	128.63	121.20
4	A	1978	C	N3-C2-O2	-5.30	118.19	121.90
4	A	1467	U	N1-C2-O2	5.30	126.51	122.80
4	A	2472	C	C5-C6-N1	5.29	123.65	121.00
5	B	113	G	C4-N9-C1'	-5.29	119.62	126.50
4	A	851	C	C5-C6-N1	5.29	123.64	121.00
4	A	2085	C	C5-C6-N1	5.28	123.64	121.00
5	B	9	G	N7-C8-N9	5.28	115.74	113.10
4	A	1382	U	C2-N1-C1'	5.28	124.03	117.70
4	A	523	U	N1-C2-O2	5.28	126.49	122.80
4	A	1298	C	C5-C6-N1	5.27	123.64	121.00
4	A	1579	C	C6-N1-C2	-5.27	118.19	120.30
4	A	910	C	C6-N1-C2	-5.27	118.19	120.30
4	A	3036	C	C2-N1-C1'	5.27	124.60	118.80
5	B	31	C	N3-C2-O2	-5.27	118.21	121.90
4	A	514	C	C5-C6-N1	5.27	123.64	121.00
4	A	2689	C	C6-N1-C1'	-5.27	114.48	120.80
4	A	2923	C	C5-C6-N1	5.27	123.63	121.00
4	A	845	C	C5-C6-N1	5.27	123.63	121.00
4	A	2269	C	C5-C6-N1	5.26	123.63	121.00
4	A	1199	U	P-O3'-C3'	5.26	126.01	119.70
4	A	2319	G	N3-C4-N9	5.26	129.16	126.00
4	A	2380	G	OP1-P-O3'	5.26	116.77	105.20
4	A	2880	U	C5-C6-N1	5.26	125.33	122.70
5	B	112	C	C5-C6-N1	5.25	123.63	121.00
4	A	1798	U	N1-C2-O2	5.25	126.47	122.80
4	A	2397	C	P-O3'-C3'	5.25	126.00	119.70
4	A	2585	U	N3-C2-O2	-5.25	118.53	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1298	C	C6-N1-C2	-5.24	118.20	120.30
5	B	10	G	P-O3'-C3'	5.24	125.99	119.70
4	A	1202	A	C4-N9-C1'	5.24	135.72	126.30
4	A	1904	C	C2-N1-C1'	5.24	124.56	118.80
4	A	1057	C	C6-N1-C2	-5.23	118.21	120.30
4	A	1900	C	C6-N1-C2	-5.23	118.21	120.30
4	A	2322	C	C5-C6-N1	5.23	123.61	121.00
4	A	1260	C	N1-C2-O2	5.23	122.04	118.90
4	A	1531	C	C2-N1-C1'	5.23	124.55	118.80
20	Q	15	ASP	CB-CG-OD1	5.23	123.00	118.30
4	A	111	U	C5-C6-N1	5.22	125.31	122.70
4	A	1102	G	C4-N9-C1'	5.22	133.29	126.50
4	A	2472	C	C2-N1-C1'	5.22	124.54	118.80
4	A	1947	U	C5-C6-N1	5.21	125.31	122.70
4	A	328	C	N1-C2-O2	5.21	122.03	118.90
4	A	1215	U	N1-C2-O2	5.21	126.45	122.80
4	A	853	C	C6-N1-C2	-5.21	118.22	120.30
4	A	3074	C	C5-C6-N1	5.21	123.60	121.00
4	A	1798	U	N3-C2-O2	-5.20	118.56	122.20
4	A	1973	C	C6-N1-C2	-5.20	118.22	120.30
4	A	2362	C	C5-C6-N1	5.19	123.60	121.00
4	A	1939	U	C5-C6-N1	5.19	125.30	122.70
4	A	2335	G	C4-N9-C1'	5.19	133.25	126.50
4	A	1409	C	C6-N1-C2	-5.19	118.22	120.30
4	A	1579	C	C6-N1-C1'	-5.19	114.58	120.80
4	A	2780	C	C2-N1-C1'	5.19	124.51	118.80
4	A	2430	C	C5-C6-N1	5.19	123.59	121.00
4	A	2532	G	N3-C4-N9	5.19	129.11	126.00
4	A	898	A	C4-N9-C1'	5.18	135.62	126.30
4	A	2477	G	C2-N3-C4	-5.18	109.31	111.90
4	A	1441	C	C2-N3-C4	5.17	122.49	119.90
4	A	543	U	C6-N1-C1'	-5.17	113.96	121.20
4	A	2939	C	C5-C6-N1	5.17	123.58	121.00
4	A	1622	G	N3-C4-C5	-5.16	126.02	128.60
4	A	43	C	C6-N1-C2	-5.16	118.24	120.30
4	A	546	G	O4'-C1'-N9	5.16	112.33	108.20
4	A	3037	C	C2-N1-C1'	5.16	124.47	118.80
4	A	1548	C	C5-C6-N1	5.16	123.58	121.00
4	A	1016	C	N1-C2-O2	5.15	121.99	118.90
4	A	1403	C	C6-N1-C1'	-5.15	114.62	120.80
4	A	1610	C	C6-N1-C2	-5.15	118.24	120.30
5	B	4	A	C8-N9-C4	-5.15	103.74	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1045	C	C6-N1-C2	-5.14	118.24	120.30
4	A	1224	G	C4-N9-C1'	5.14	133.19	126.50
4	A	154	C	C6-N1-C2	-5.14	118.24	120.30
4	A	197	C	C2-N1-C1'	5.14	124.46	118.80
8	E	122	ASP	CB-CG-OD2	5.14	122.93	118.30
4	A	2585	U	N1-C2-O2	5.14	126.40	122.80
4	A	1513	C	C2-N1-C1'	5.14	124.45	118.80
4	A	742	G	N3-C4-N9	5.13	129.08	126.00
4	A	2592	C	C6-N1-C2	-5.13	118.25	120.30
4	A	1640	A	C4-N9-C1'	5.13	135.53	126.30
4	A	853	C	N1-C2-O2	5.12	121.97	118.90
4	A	999	C	C6-N1-C2	-5.12	118.25	120.30
4	A	1441	C	C5-C6-N1	5.12	123.56	121.00
4	A	2022	U	N3-C2-O2	-5.12	118.62	122.20
4	A	2260	C	N1-C2-O2	5.12	121.97	118.90
4	A	498	G	C6-C5-N7	-5.12	127.33	130.40
4	A	1198	C	C6-N1-C2	-5.11	118.25	120.30
4	A	1874	C	C5-C6-N1	5.11	123.56	121.00
4	A	2418	U	N3-C2-O2	-5.11	118.62	122.20
4	A	709	U	C6-N1-C1'	-5.11	114.05	121.20
4	A	514	C	C2-N1-C1'	5.11	124.42	118.80
4	A	1521	C	C6-N1-C2	-5.10	118.26	120.30
4	A	2699	C	C5-C6-N1	5.10	123.55	121.00
4	A	2880	U	C2-N1-C1'	5.10	123.82	117.70
4	A	2884	A	C2-N3-C4	5.10	113.15	110.60
4	A	7	U	N1-C2-O2	5.10	126.37	122.80
4	A	571	A	O4'-C1'-N9	5.09	112.28	108.20
4	A	2218	C	C6-N1-C2	-5.09	118.26	120.30
4	A	472	C	C6-N1-C1'	-5.09	114.69	120.80
4	A	1001	C	C5-C6-N1	5.09	123.55	121.00
4	A	2571	C	N1-C2-O2	5.09	121.95	118.90
4	A	1171	C	C2-N3-C4	5.08	122.44	119.90
4	A	2761	U	N3-C2-O2	-5.08	118.64	122.20
4	A	757	G	O4'-C1'-N9	5.08	112.26	108.20
4	A	205	U	C2-N1-C1'	5.07	123.79	117.70
4	A	3046	C	O4'-C1'-N1	5.07	112.26	108.20
4	A	2514	G	N3-C4-N9	5.07	129.04	126.00
4	A	142	C	C6-N1-C2	-5.07	118.27	120.30
4	A	952	C	C6-N1-C2	-5.07	118.27	120.30
4	A	2328	G	P-O3'-C3'	5.07	125.78	119.70
4	A	3023	G	C8-N9-C4	-5.06	104.38	106.40
4	A	1225	G	C5-N7-C8	-5.06	101.77	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2289	C	C5-C6-N1	5.06	123.53	121.00
4	A	1045	C	N1-C2-O2	5.05	121.93	118.90
4	A	2155	U	N3-C2-O2	-5.05	118.66	122.20
4	A	2418	U	C2-N1-C1'	5.05	123.76	117.70
4	A	1102	G	N3-C4-N9	5.05	129.03	126.00
4	A	1460	C	C2-N1-C1'	5.05	124.35	118.80
4	A	1618	C	C6-N1-C2	-5.05	118.28	120.30
4	A	467	C	C6-N1-C2	-5.04	118.28	120.30
4	A	1382	U	N3-C2-O2	-5.04	118.67	122.20
4	A	2633	G	N3-C4-N9	5.04	129.03	126.00
5	B	38	C	N1-C2-O2	5.04	121.92	118.90
4	A	1893	C	C5-C6-N1	5.04	123.52	121.00
4	A	1610	C	N3-C2-O2	-5.04	118.37	121.90
3	4	267	GLY	N-CA-C	-5.04	100.51	113.10
5	B	111	C	N1-C2-O2	5.04	121.92	118.90
4	A	1887	A	C2-N3-C4	5.03	113.12	110.60
4	A	2077	C	C5-C6-N1	5.03	123.52	121.00
4	A	2939	C	C6-N1-C2	-5.03	118.29	120.30
4	A	2249	G	N3-C4-N9	5.03	129.02	126.00
4	A	281	C	C6-N1-C2	-5.03	118.29	120.30
4	A	630	U	C2-N1-C1'	5.02	123.73	117.70
4	A	2698	C	C6-N1-C2	-5.02	118.29	120.30
4	A	2086	U	C5-C6-N1	5.02	125.21	122.70
4	A	2267	C	C5-C6-N1	5.01	123.51	121.00
4	A	366	G	N3-C4-N9	5.01	129.00	126.00
4	A	2132	U	N3-C2-O2	-5.01	118.69	122.20
4	A	1697	U	C2-N1-C1'	5.01	123.71	117.70
4	A	1993	G	C8-N9-C1'	-5.01	120.49	127.00
5	B	10	G	OP1-P-O3'	5.01	116.21	105.20
4	A	836	G	C4-N9-C1'	5.00	133.01	126.50
4	A	3016	C	N1-C2-O2	5.00	121.90	118.90
4	A	1034	U	N1-C2-O2	5.00	126.30	122.80

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	F	68	THR	Peptide
10	G	46	ALA	Peptide
10	G	52	VAL	Peptide
11	H	137	HIS	Peptide
12	I	52	ALA	Peptide

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Mol	Chain	Res	Type	Group
12	I	53	LYS	Peptide
13	J	54	ASN	Peptide
18	O	57	LYS	Peptide
19	P	102	PHE	Peptide
19	P	25	LEU	Peptide
19	P	5	PRO	Peptide
19	P	80	HIS	Peptide
26	W	118	ALA	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	474	0	500	2	0
2	3	189	0	205	3	0
3	4	3228	0	3284	515	0
4	A	66981	0	33700	293	0
5	B	2522	0	1285	20	0
6	C	2110	0	2165	28	0
7	D	1587	0	1630	12	0
8	E	1569	0	1607	13	0
9	F	1445	0	1476	23	0
10	G	1348	0	1399	20	0
11	H	1018	0	988	19	0
12	I	918	0	959	29	0
13	J	990	0	1021	26	0
14	K	1130	0	1167	8	0
15	L	938	0	1000	7	0
16	M	1078	0	1151	8	0
17	N	1092	0	1128	9	0
18	O	928	0	972	5	0
19	P	956	0	991	42	0
20	Q	907	0	938	8	0
21	R	988	0	1038	11	0
22	S	754	0	802	7	0
23	T	873	0	909	8	0
24	U	756	0	802	2	0
25	V	732	0	782	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	W	1428	0	1443	11	0
27	X	586	0	601	7	0
28	Y	470	0	482	4	0
29	Z	531	0	541	3	0
30	b	423	0	463	0	0
31	c	405	0	411	0	0
32	d	377	0	411	0	0
33	e	502	0	541	0	0
34	f	299	0	324	0	0
35	g	364	0	352	0	0
36	4	32	0	14	15	0
All	All	100928	0	67482	1038	0

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

All (1038) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:445:THR:CG2	3:4:450:ARG:HB2	1.86	1.06
3:4:202:GLY:HA3	4:A:2676:C:C4'	1.86	1.05
3:4:354:VAL:HG11	3:4:361:PRO:HG3	1.38	1.04
3:4:426:ARG:HG3	3:4:429:LEU:HB2	1.38	1.04
3:4:85:LEU:HD11	3:4:106:LEU:HD21	1.40	1.02
3:4:261:LEU:HD11	3:4:392:VAL:HG11	1.40	1.00
3:4:202:GLY:HA3	4:A:2676:C:H4'	1.40	0.99
3:4:102:LYS:HG2	4:A:2132:U:H5'	1.43	0.98
3:4:85:LEU:CD1	3:4:106:LEU:HD21	1.95	0.97
3:4:395:ARG:HH21	36:4:501:GCP:C2	1.79	0.96
3:4:288:GLU:HG3	3:4:292:GLY:HA2	1.46	0.94
3:4:288:GLU:CG	3:4:292:GLY:HA2	1.97	0.94
3:4:177:ARG:HA	3:4:183:MET:SD	2.08	0.94
3:4:48:ARG:HB3	3:4:115:ALA:HA	1.50	0.93
3:4:250:ILE:CD1	3:4:258:LYS:HA	1.98	0.93
3:4:373:ALA:CB	36:4:501:GCP:HN1	1.82	0.92
4:A:1209:G:H1	4:A:1219:U:H3	1.18	0.91
3:4:42:ARG:HH12	3:4:44:LEU:HB2	1.35	0.91
3:4:181:GLU:HA	3:4:184:SER:CB	2.00	0.90
3:4:445:THR:HG23	3:4:450:ARG:HB2	1.50	0.90
4:A:2329:G:H1	4:A:2406:U:H3	1.17	0.90
3:4:173:LEU:HD13	3:4:215:ILE:HG21	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:379:LEU:HG	3:4:383:ARG:HD2	1.55	0.88
3:4:187:ALA:HA	4:A:2826:A:C5	2.08	0.88
3:4:354:VAL:HG13	3:4:359:ILE:HG13	1.56	0.87
3:4:181:GLU:HA	3:4:184:SER:HB2	1.53	0.87
3:4:186:GLN:HB3	3:4:207:LYS:HZ3	1.37	0.87
3:4:384:ARG:HG2	3:4:385:ALA:N	1.90	0.87
3:4:227:ARG:NE	3:4:227:ARG:HA	1.90	0.85
3:4:286:ARG:HB2	4:A:2697:U:O2'	1.76	0.85
3:4:434:HIS:HB3	4:A:1185:A:H1'	1.59	0.85
3:4:426:ARG:HA	3:4:429:LEU:HD23	1.56	0.85
3:4:383:ARG:HH21	3:4:391:PHE:HE1	1.24	0.85
19:P:50:GLN:HA	19:P:63:ALA:HB3	1.59	0.84
3:4:82:LEU:HD13	3:4:113:THR:HB	1.59	0.84
3:4:371:ILE:HA	3:4:374:ALA:HB2	1.60	0.83
3:4:271:LEU:HD22	3:4:278:ALA:HB1	1.61	0.83
3:4:350:ILE:O	3:4:353:VAL:HG22	1.79	0.82
3:4:373:ALA:HB3	36:4:501:GCP:HN1	1.39	0.82
3:4:432:ARG:HB3	3:4:436:ASP:HB2	1.61	0.82
3:4:85:LEU:HD21	3:4:106:LEU:CD1	2.09	0.82
3:4:228:ASP:O	3:4:231:LYS:HG2	1.80	0.82
3:4:46:LEU:HD12	3:4:117:THR:CG2	2.09	0.82
3:4:294:PRO:HB3	3:4:296:VAL:HG23	1.62	0.81
3:4:445:THR:HG21	3:4:450:ARG:HB2	1.61	0.81
3:4:250:ILE:HD11	3:4:258:LYS:HA	1.64	0.80
3:4:326:ASP:HB3	3:4:412:GLU:OE1	1.81	0.80
3:4:461:ALA:HB3	3:4:463:LEU:HD13	1.62	0.80
3:4:187:ALA:HA	4:A:2826:A:C4	2.16	0.80
3:4:253:TYR:HE1	3:4:332:VAL:HG12	1.45	0.80
3:4:227:ARG:HA	3:4:227:ARG:HE	1.46	0.79
3:4:250:ILE:HD13	3:4:258:LYS:HA	1.63	0.79
3:4:251:VAL:HG22	3:4:252:GLY:H	1.47	0.79
4:A:2140:A:H5'	4:A:2141:U:C5	2.18	0.79
4:A:2367:G:N2	4:A:2370:A:C5	2.50	0.79
3:4:49:VAL:HG12	3:4:117:THR:OG1	1.83	0.79
3:4:294:PRO:O	3:4:295:PHE:C	2.19	0.79
3:4:327:LEU:C	3:4:328:LEU:HD12	2.04	0.78
3:4:293:ARG:HH22	3:4:414:THR:HA	1.47	0.78
3:4:372:ASP:C	3:4:374:ALA:H	1.86	0.78
3:4:395:ARG:NH2	36:4:501:GCP:N3	2.30	0.78
3:4:420:VAL:HA	3:4:466:TYR:HD1	1.47	0.78
3:4:426:ARG:HE	3:4:430:VAL:HG13	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1566:A:H61	4:A:1606:G:N2	1.83	0.77
3:4:271:LEU:CD2	3:4:278:ALA:HB1	2.15	0.76
4:A:2367:G:C2	4:A:2370:A:N7	2.53	0.76
3:4:42:ARG:NH1	3:4:44:LEU:HB2	1.99	0.76
3:4:107:ARG:O	3:4:110:VAL:HG12	1.84	0.76
3:4:381:GLN:O	3:4:384:ARG:HD3	1.86	0.76
3:4:420:VAL:HG22	3:4:421:THR:N	2.02	0.75
3:4:456:PRO:HB2	3:4:459:LEU:HD23	1.69	0.75
3:4:382:LEU:HB3	3:4:386:LEU:HD12	1.68	0.75
12:I:37:ALA:O	12:I:41:ARG:HB3	1.87	0.74
3:4:371:ILE:HG22	3:4:372:ASP:H	1.52	0.74
3:4:344:ASN:O	3:4:348:THR:HG23	1.86	0.74
3:4:250:ILE:HG22	3:4:298:THR:O	1.88	0.74
3:4:257:GLY:O	36:4:501:GCP:O3A	2.05	0.74
3:4:443:GLU:HG2	3:4:452:LYS:HD3	1.69	0.73
3:4:366:LEU:HD11	3:4:387:PRO:HD2	1.69	0.73
3:4:173:LEU:HD13	3:4:215:ILE:CG2	2.19	0.73
3:4:379:LEU:O	3:4:383:ARG:HG3	1.88	0.72
3:4:223:ARG:HA	3:4:226:ILE:HD11	1.71	0.72
3:4:420:VAL:HG22	3:4:421:THR:H	1.52	0.72
3:4:443:GLU:HG2	3:4:452:LYS:CD	2.18	0.72
3:4:300:THR:HB	3:4:318:THR:HG23	1.70	0.72
3:4:395:ARG:HG2	3:4:396:THR:H	1.54	0.72
3:4:45:ARG:O	3:4:46:LEU:HD13	1.88	0.72
3:4:288:GLU:CB	3:4:292:GLY:HA2	2.19	0.72
3:4:383:ARG:HB3	3:4:383:ARG:NH1	2.03	0.72
3:4:339:PRO:HG2	3:4:382:LEU:HD21	1.72	0.72
3:4:147:ILE:HD11	3:4:151:PHE:CE2	2.24	0.72
3:4:422:ILE:HG23	3:4:429:LEU:HG	1.71	0.72
19:P:42:ARG:HH11	19:P:109:TYR:H	1.38	0.72
3:4:153:GLN:HG3	3:4:154:HIS:HD2	1.56	0.71
3:4:424:TYR:CZ	3:4:447:ALA:HA	2.24	0.71
3:4:251:VAL:HG22	3:4:252:GLY:N	2.04	0.71
3:4:87:GLN:HG3	4:A:2133:G:H5''	1.71	0.71
3:4:213:ARG:O	3:4:217:GLU:HG3	1.90	0.71
3:4:288:GLU:HG3	3:4:292:GLY:CA	2.20	0.71
3:4:366:LEU:HD23	3:4:366:LEU:H	1.56	0.71
3:4:87:GLN:NE2	4:A:2133:G:H8	1.89	0.70
3:4:102:LYS:O	3:4:106:LEU:HD23	1.90	0.70
3:4:181:GLU:HA	3:4:184:SER:HB3	1.73	0.70
4:A:1566:A:N6	4:A:1606:G:H21	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1158:U:H3	4:A:1232:G:H1	1.37	0.70
3:4:199:GLY:C	3:4:201:ARG:H	1.94	0.70
19:P:73:ILE:HG13	19:P:75:GLY:H	1.56	0.70
3:4:102:LYS:HD3	4:A:2133:G:O5'	1.91	0.70
3:4:426:ARG:C	3:4:428:ASP:H	1.93	0.70
3:4:45:ARG:C	3:4:46:LEU:HD22	2.11	0.70
3:4:50:VAL:CG2	3:4:118:VAL:HG22	2.22	0.69
3:4:373:ALA:HB3	36:4:501:GCP:N1	2.08	0.69
3:4:263:ASN:HD21	3:4:270:VAL:H	1.41	0.69
3:4:147:ILE:HG21	3:4:308:PRO:HG3	1.74	0.69
7:D:63:ILE:HG22	7:D:65:PRO:HD2	1.73	0.69
3:4:199:GLY:CA	3:4:201:ARG:HD2	2.23	0.69
3:4:340:LEU:H	3:4:340:LEU:HD22	1.58	0.68
4:A:2413:G:H2'	4:A:2414:G:H8	1.58	0.68
3:4:430:VAL:O	3:4:431:ALA:C	2.31	0.68
5:B:112:C:H3'	5:B:113:G:H4'	1.73	0.68
4:A:365:U:H3	4:A:437:G:H1	1.41	0.68
3:4:260:SER:OG	3:4:394:ALA:HB1	1.94	0.68
3:4:311:LEU:HD23	3:4:312:VAL:H	1.58	0.68
3:4:327:LEU:HD23	3:4:328:LEU:N	2.09	0.68
3:4:46:LEU:HD12	3:4:117:THR:HG21	1.76	0.67
3:4:349:VAL:O	3:4:353:VAL:HG13	1.94	0.67
3:4:371:ILE:HB	3:4:391:PHE:HA	1.75	0.67
3:4:199:GLY:HA2	3:4:201:ARG:CZ	2.24	0.67
3:4:436:ASP:HB3	3:4:439:VAL:HG13	1.76	0.67
3:4:271:LEU:HD23	3:4:273:GLU:H	1.57	0.67
3:4:432:ARG:HA	3:4:435:THR:HG23	1.75	0.67
9:F:124:LEU:HB2	9:F:185:LYS:HG2	1.74	0.67
3:4:432:ARG:HB3	3:4:436:ASP:CB	2.24	0.67
25:V:43:LYS:HB3	25:V:59:ILE:HA	1.77	0.67
4:A:2140:A:H5'	4:A:2141:U:H5	1.59	0.67
3:4:202:GLY:N	3:4:203:PRO:HD2	2.10	0.66
3:4:288:GLU:HB2	3:4:292:GLY:HA2	1.78	0.66
3:4:455:VAL:HB	3:4:460:ALA:HB3	1.75	0.66
3:4:422:ILE:HG21	3:4:426:ARG:NH1	2.10	0.66
3:4:370:LYS:O	3:4:374:ALA:HA	1.96	0.66
3:4:372:ASP:C	3:4:374:ALA:N	2.49	0.66
4:A:2367:G:C2	4:A:2370:A:C5	2.84	0.66
3:4:307:LEU:HD13	3:4:312:VAL:HG21	1.76	0.66
3:4:271:LEU:HD21	3:4:273:GLU:HB2	1.78	0.66
4:A:1209:G:N1	4:A:1219:U:N3	2.39	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:84:ALA:HA	11:H:91:LEU:HA	1.78	0.66
4:A:2474:G:H5''	4:A:2474:G:N3	2.11	0.65
3:4:461:ALA:HB3	3:4:463:LEU:CD1	2.26	0.65
3:4:445:THR:HG21	3:4:450:ARG:CB	2.27	0.65
4:A:1636:A:H62	4:A:1802:G:H21	1.45	0.65
3:4:85:LEU:HD21	3:4:106:LEU:HD13	1.77	0.65
3:4:371:ILE:HG22	3:4:372:ASP:N	2.11	0.65
3:4:148:LEU:HD12	3:4:148:LEU:O	1.96	0.65
3:4:432:ARG:HH21	3:4:459:LEU:HA	1.62	0.65
4:A:2134:G:N2	4:A:2146:A:O2'	2.29	0.65
4:A:2335:G:N7	4:A:2392:A:N6	2.45	0.65
3:4:379:LEU:CG	3:4:383:ARG:HD2	2.28	0.64
3:4:186:GLN:HB3	3:4:207:LYS:NZ	2.10	0.64
3:4:237:ARG:O	3:4:237:ARG:HG3	1.97	0.64
3:4:199:GLY:HA3	3:4:201:ARG:HD2	1.79	0.64
4:A:347:U:H2'	4:A:348:G:H8	1.63	0.64
4:A:2034:G:OP1	6:C:88:ARG:NH2	2.30	0.64
3:4:202:GLY:O	3:4:203:PRO:C	2.35	0.64
3:4:445:THR:HG21	3:4:450:ARG:HG3	1.80	0.63
11:H:118:GLN:HG3	11:H:120:ALA:H	1.63	0.63
3:4:374:ALA:C	3:4:376:GLY:H	2.00	0.63
3:4:426:ARG:NE	3:4:430:VAL:HG13	2.14	0.63
4:A:2136:A:N6	4:A:2139:U:C4	2.67	0.63
3:4:443:GLU:CG	3:4:452:LYS:HD3	2.28	0.63
13:J:135:ARG:NH1	13:J:136:SER:OG	2.32	0.63
3:4:424:TYR:OH	3:4:447:ALA:HA	1.97	0.63
9:F:150:VAL:HA	9:F:153:ILE:HD12	1.81	0.62
4:A:2137:A:H4'	4:A:2142:A:N1	2.13	0.62
3:4:323:VAL:HG21	3:4:357:TYR:CD1	2.34	0.62
3:4:46:LEU:O	3:4:47:GLU:HB2	1.99	0.62
3:4:263:ASN:OD1	3:4:270:VAL:HG22	1.99	0.62
4:A:747:A:N6	4:A:768:G:O2'	2.33	0.62
3:4:424:TYR:HB3	13:J:31:GLY:O	2.00	0.62
4:A:2363:A:H61	4:A:2374:U:H3	1.47	0.62
3:4:165:SER:HA	3:4:168:GLN:HG3	1.82	0.61
3:4:171:TYR:HB2	3:4:310:GLN:OE1	1.99	0.61
4:A:572:C:H2'	25:V:46:ALA:HA	1.82	0.61
3:4:442:THR:HG23	3:4:442:THR:O	2.00	0.61
12:I:1:MET:SD	12:I:6:LYS:NZ	2.73	0.61
19:P:39:VAL:O	19:P:49:VAL:HG13	2.00	0.61
4:A:2137:A:O3'	4:A:2138:C:H4'	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:85:LEU:HD21	3:4:106:LEU:HD11	1.82	0.61
3:4:408:GLY:O	3:4:411:VAL:HG22	2.00	0.61
4:A:1273:G:OP2	21:R:58:ARG:NH1	2.33	0.61
4:A:1599:U:H5''	4:A:1600:G:H8	1.66	0.61
4:A:1825:C:N4	4:A:1840:G:OP2	2.32	0.61
3:4:76:THR:CG2	3:4:150:ILE:HD11	2.31	0.61
3:4:319:LEU:O	3:4:322:VAL:HG12	2.01	0.61
19:P:42:ARG:NH1	19:P:109:TYR:O	2.34	0.61
3:4:245:ILE:CG2	3:4:294:PRO:HG2	2.30	0.61
3:4:444:HIS:CD2	3:4:445:THR:H	2.18	0.61
3:4:148:LEU:HA	3:4:311:LEU:HD13	1.83	0.61
6:C:136:ILE:HG21	6:C:142:ILE:HD11	1.82	0.61
3:4:147:ILE:O	3:4:150:ILE:HG22	2.01	0.61
4:A:570:U:O4'	25:V:44:HIS:NE2	2.34	0.61
3:4:383:ARG:HB3	3:4:383:ARG:HH11	1.64	0.60
4:A:325:U:O2	4:A:450:G:C2	2.54	0.60
18:O:10:LEU:HB2	18:O:17:GLN:HG3	1.84	0.60
3:4:50:VAL:HG23	3:4:118:VAL:HG22	1.83	0.60
3:4:117:THR:HA	3:4:139:LYS:HB2	1.82	0.60
4:A:1187:A:O2'	4:A:1191:A:N1	2.33	0.60
4:A:1611:A:H2	6:C:134:ARG:HH21	1.47	0.60
3:4:371:ILE:HD12	3:4:390:VAL:O	2.00	0.60
3:4:443:GLU:HG2	3:4:452:LYS:CG	2.31	0.60
4:A:1863:G:H5''	4:A:1864:U:H5'	1.83	0.60
4:A:2014:G:HO2'	6:C:257:THR:HG1	1.44	0.60
3:4:340:LEU:HD22	3:4:340:LEU:N	2.16	0.60
3:4:354:VAL:HG13	3:4:359:ILE:CG1	2.29	0.60
4:A:2160:A:H61	4:A:2187:U:H3	1.48	0.60
26:W:28:ARG:NH1	26:W:93:GLN:O	2.34	0.60
4:A:2245:C:OP1	21:R:25:ARG:NH1	2.35	0.60
28:Y:17:SER:HB3	28:Y:27:ARG:HD2	1.83	0.60
3:4:353:VAL:CG2	3:4:354:VAL:N	2.65	0.60
3:4:366:LEU:HD21	3:4:387:PRO:HB2	1.82	0.60
19:P:43:SER:HB2	19:P:47:ILE:HG22	1.84	0.60
19:P:84:VAL:HG13	19:P:116:LEU:HD13	1.83	0.60
4:A:1156:A:H2'	4:A:1157:G:C8	2.37	0.60
18:O:11:GLY:O	18:O:16:HIS:ND1	2.34	0.60
4:A:587:G:N1	4:A:590:A:OP2	2.35	0.59
3:4:167:ALA:O	3:4:170:GLU:HG2	2.03	0.59
3:4:199:GLY:C	3:4:201:ARG:N	2.55	0.59
7:D:7:LEU:H	7:D:34:ASN:HD21	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:51:ILE:HD11	10:G:73:ILE:HD12	1.84	0.59
3:4:294:PRO:O	3:4:296:VAL:N	2.35	0.59
3:4:180:GLY:O	3:4:184:SER:HB2	2.01	0.59
15:L:115:VAL:HG13	15:L:121:VAL:HG21	1.84	0.59
4:A:1001:C:N4	4:A:1004:C:OP2	2.34	0.59
3:4:291:ASP:OD2	3:4:438:HIS:HB3	2.01	0.59
3:4:392:VAL:HG13	3:4:400:LEU:CD2	2.32	0.59
3:4:426:ARG:HA	3:4:429:LEU:CD2	2.30	0.59
4:A:861:U:O4	7:D:142:GLN:NE2	2.35	0.59
5:B:9:G:H5'	5:B:10:G:H2'	1.84	0.59
12:I:20:SER:OG	12:I:21:THR:N	2.36	0.59
3:4:153:GLN:HG3	3:4:154:HIS:CD2	2.37	0.59
3:4:219:MET:O	3:4:223:ARG:HG3	2.03	0.59
6:C:163:ILE:HG22	6:C:178:PRO:HD3	1.82	0.59
2:3:22:PRO:HB3	4:A:1102:G:H2'	1.84	0.59
3:4:436:ASP:HB3	3:4:439:VAL:HG22	1.85	0.59
4:A:896:A:OP1	6:C:218:ARG:NH2	2.35	0.59
4:A:1582:C:N4	4:A:1589:G:O6	2.35	0.59
5:B:50:C:H5''	19:P:78:LYS:HB3	1.84	0.59
3:4:46:LEU:HD12	3:4:117:THR:HG22	1.84	0.58
3:4:243:SER:O	3:4:244:GLU:C	2.40	0.58
3:4:295:PHE:CG	3:4:295:PHE:O	2.55	0.58
4:A:1555:A:N6	4:A:1617:C:O2	2.36	0.58
4:A:2131:G:O6	4:A:2148:C:N4	2.36	0.58
4:A:1198:C:H41	4:A:1205:G:H5''	1.68	0.58
6:C:66:ASP:OD1	6:C:103:ARG:NH1	2.36	0.58
4:A:1209:G:O6	4:A:1219:U:C4	2.56	0.58
29:Z:45:ARG:HH12	29:Z:48:ARG:HH21	1.52	0.58
3:4:420:VAL:HG23	3:4:466:TYR:HA	1.84	0.58
4:A:325:U:O2	4:A:450:G:N2	2.36	0.58
3:4:202:GLY:HA3	4:A:2676:C:O4'	2.02	0.58
3:4:327:LEU:HA	3:4:363:PRO:O	2.03	0.58
4:A:2385:G:OP1	4:A:2396:A:N6	2.36	0.58
3:4:106:LEU:HA	3:4:109:VAL:HG22	1.85	0.58
3:4:150:ILE:HG23	3:4:151:PHE:HD2	1.69	0.58
3:4:293:ARG:NH2	3:4:414:THR:HA	2.19	0.58
4:A:1177:G:H21	13:J:113:THR:HB	1.68	0.58
13:J:13:LEU:HD13	13:J:15:ILE:HG22	1.86	0.58
3:4:311:LEU:HD23	3:4:312:VAL:N	2.19	0.57
3:4:329:ILE:O	3:4:329:ILE:HG22	2.04	0.57
3:4:432:ARG:HE	3:4:459:LEU:HD12	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:289:A:N6	4:A:300:G:O6	2.37	0.57
3:4:443:GLU:HG2	3:4:452:LYS:HG3	1.86	0.57
3:4:353:VAL:HG23	3:4:354:VAL:N	2.20	0.57
4:A:2135:U:C5	4:A:2137:A:C8	2.92	0.57
4:A:2967:C:O2'	10:G:151:ARG:NH1	2.37	0.57
19:P:42:ARG:H	19:P:106:GLY:HA3	1.70	0.57
17:N:65:TRP:HB2	17:N:105:GLU:HB2	1.87	0.57
3:4:100:SER:OG	4:A:2131:G:H4'	2.05	0.57
3:4:283:THR:HG23	3:4:299:ASP:HB3	1.86	0.57
3:4:107:ARG:HD3	3:4:135:ALA:O	2.04	0.57
3:4:242:ARG:O	3:4:243:SER:C	2.43	0.57
3:4:123:GLU:C	3:4:124:LEU:HD12	2.24	0.57
3:4:367:VAL:CG1	3:4:392:VAL:HG21	2.35	0.57
4:A:730:G:H2'	16:M:113:LEU:HD13	1.87	0.57
4:A:2286:A:H2	4:A:2727:A:H62	1.52	0.57
4:A:2390:U:O2	4:A:2392:A:N6	2.38	0.57
4:A:2532:G:H3'	4:A:2533:C:H2'	1.85	0.57
9:F:55:LYS:HA	9:F:58:ASN:HD22	1.70	0.57
13:J:74:THR:HG23	13:J:83:LYS:HD3	1.86	0.57
4:A:759:G:H1	27:X:64:PRO:HB3	1.69	0.57
6:C:108:PRO:HD2	6:C:111:LEU:HD22	1.87	0.57
29:Z:11:ARG:NH1	29:Z:63:GLU:OE1	2.38	0.57
4:A:1272:C:OP1	21:R:92:ARG:NH2	2.37	0.56
9:F:129:PHE:HE1	9:F:136:THR:H	1.54	0.56
3:4:267:GLY:O	3:4:268:ALA:HB3	2.05	0.56
3:4:371:ILE:O	3:4:372:ASP:HB2	2.04	0.56
3:4:379:LEU:HD21	3:4:391:PHE:CE2	2.39	0.56
4:A:1541:G:OP2	4:A:1629:G:N2	2.39	0.56
4:A:2335:G:OP2	4:A:2338:G:N1	2.37	0.56
17:N:35:GLN:OE1	17:N:130:ARG:NH2	2.39	0.56
3:4:47:GLU:HA	3:4:79:SER:CA	2.35	0.56
3:4:438:HIS:O	3:4:439:VAL:C	2.42	0.56
3:4:443:GLU:O	3:4:451:ILE:HD13	2.05	0.56
4:A:1172:A:N3	12:I:29:ARG:NH1	2.53	0.56
4:A:1398:G:N2	4:A:1401:A:OP2	2.37	0.56
3:4:263:ASN:ND2	3:4:270:VAL:H	2.02	0.56
4:A:2015:U:OP2	6:C:272:ARG:NH2	2.38	0.56
4:A:2802:G:H21	7:D:135:GLN:HE21	1.54	0.56
5:B:7:G:O2'	19:P:37:ARG:NH2	2.39	0.56
3:4:436:ASP:HB3	3:4:439:VAL:CG1	2.35	0.56
3:4:61:ALA:HA	3:4:64:GLU:OE2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2476:G:H2'	4:A:2477:G:H8	1.70	0.56
5:B:43:C:H5'	9:F:71:LYS:HD2	1.86	0.56
3:4:132:LEU:O	3:4:136:VAL:HG22	2.06	0.56
3:4:393:SER:O	36:4:501:GCP:N7	2.39	0.56
4:A:1556:A:H2	4:A:1615:G:H22	1.52	0.56
13:J:34:GLY:O	13:J:66:ARG:NH1	2.39	0.56
4:A:2043:C:O2'	4:A:2195:U:OP2	2.24	0.56
3:4:47:GLU:HA	3:4:79:SER:HA	1.88	0.56
4:A:1112:C:O2	22:S:12:LYS:NZ	2.37	0.56
4:A:2367:G:N3	4:A:2370:A:N7	2.54	0.56
19:P:46:HIS:NE2	19:P:65:SER:O	2.39	0.56
3:4:47:GLU:HA	3:4:79:SER:HB3	1.87	0.56
3:4:327:LEU:HD21	3:4:329:ILE:CD1	2.35	0.56
4:A:2035:U:OP2	6:C:157:ARG:NH1	2.39	0.56
3:4:43:GLN:HA	3:4:43:GLN:NE2	2.20	0.55
3:4:183:MET:HA	3:4:186:GLN:HB2	1.86	0.55
4:A:365:U:O2	4:A:437:G:N2	2.37	0.55
4:A:1224:G:O2'	12:I:54:ASN:ND2	2.40	0.55
5:B:112:C:N4	5:B:113:G:N3	2.54	0.55
19:P:50:GLN:HA	19:P:63:ALA:CB	2.34	0.55
3:4:420:VAL:CG2	3:4:466:TYR:HA	2.36	0.55
3:4:76:THR:HG21	3:4:150:ILE:HD11	1.88	0.55
3:4:393:SER:C	3:4:395:ARG:H	2.10	0.55
3:4:426:ARG:C	3:4:428:ASP:N	2.59	0.55
15:L:50:GLY:O	15:L:53:LYS:NZ	2.39	0.55
4:A:573:C:H41	25:V:47:VAL:HB	1.72	0.55
4:A:652:C:O2'	21:R:48:ARG:NH1	2.40	0.55
10:G:29:PRO:HD3	10:G:80:VAL:HA	1.89	0.55
4:A:1209:G:O6	4:A:1219:U:O4	2.24	0.55
4:A:1540:U:O2	4:A:1632:G:O6	2.25	0.55
3:4:202:GLY:O	3:4:204:GLY:N	2.40	0.55
3:4:246:PRO:CD	3:4:293:ARG:HB3	2.37	0.55
4:A:2136:A:N3	4:A:2136:A:H2'	2.22	0.55
3:4:167:ALA:HB2	3:4:311:LEU:HA	1.89	0.55
3:4:187:ALA:CA	4:A:2826:A:C5	2.86	0.55
3:4:333:ASP:OD2	3:4:336:ASP:HB2	2.07	0.55
3:4:432:ARG:HA	3:4:435:THR:O	2.07	0.55
4:A:1181:G:N2	13:J:136:SER:O	2.39	0.55
4:A:1455:U:OP1	24:U:19:LYS:NZ	2.39	0.55
4:A:3102:U:O2	18:O:45:ARG:NH2	2.39	0.55
15:L:63:VAL:HG12	15:L:106:LEU:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:370:LYS:HE3	36:4:501:GCP:HI'	1.89	0.55
4:A:615:A:OP2	14:K:116:ARG:NH1	2.40	0.55
3:4:441:ALA:H	3:4:453:ALA:CB	2.20	0.55
3:4:422:ILE:O	3:4:448:GLY:HA3	2.07	0.55
3:4:444:HIS:CG	3:4:445:THR:H	2.25	0.55
4:A:1710:A:N6	4:A:1716:A:N7	2.54	0.55
3:4:253:TYR:CD1	3:4:342:GLN:HB3	2.42	0.54
4:A:889:A:OP1	6:C:48:ARG:NH1	2.40	0.54
4:A:3066:C:H5''	20:Q:52:GLY:HA3	1.89	0.54
4:A:1122:C:H2'	4:A:1129:G:H2'	1.89	0.54
4:A:2538:A:OP1	9:F:95:ARG:NH2	2.40	0.54
3:4:340:LEU:H	3:4:340:LEU:CD2	2.20	0.54
3:4:445:THR:HG21	3:4:450:ARG:CG	2.37	0.54
4:A:1562:C:H2'	4:A:1563:A:C8	2.41	0.54
3:4:444:HIS:CG	3:4:445:THR:N	2.74	0.54
4:A:2137:A:H3'	4:A:2137:A:N3	2.21	0.54
12:I:3:LYS:O	12:I:7:ALA:HB3	2.08	0.54
3:4:271:LEU:CD2	3:4:273:GLU:H	2.21	0.54
4:A:2323:G:O6	4:A:2412:U:C4	2.61	0.54
4:A:3070:G:O2'	4:A:3087:G:N2	2.41	0.54
19:P:22:HIS:HA	19:P:105:GLY:HA2	1.88	0.54
3:4:159:GLU:HG3	3:4:229:MET:SD	2.47	0.54
3:4:430:VAL:O	3:4:432:ARG:N	2.40	0.54
19:P:40:VAL:HG23	19:P:106:GLY:H	1.73	0.54
20:Q:48:ARG:HD2	20:Q:50:GLN:HB2	1.88	0.54
3:4:292:GLY:O	3:4:293:ARG:C	2.43	0.54
16:M:91:GLY:H	16:M:122:VAL:HG23	1.73	0.54
23:T:25:ARG:HA	23:T:28:ILE:HG12	1.89	0.54
3:4:251:VAL:CG2	3:4:252:GLY:H	2.20	0.54
3:4:374:ALA:C	3:4:376:GLY:N	2.62	0.54
4:A:1552:A:O2'	4:A:1618:C:N4	2.40	0.54
3:4:148:LEU:HD12	3:4:148:LEU:C	2.27	0.54
3:4:294:PRO:CB	3:4:296:VAL:HG23	2.34	0.54
3:4:323:VAL:HG21	3:4:357:TYR:CE1	2.43	0.54
4:A:1181:G:O2'	13:J:91:SER:O	2.26	0.54
4:A:1199:U:OP1	4:A:1201:G:N2	2.41	0.54
3:4:436:ASP:CB	3:4:439:VAL:HG13	2.37	0.54
4:A:1560:U:O2	6:C:134:ARG:NH2	2.41	0.54
4:A:2754:G:N7	10:G:173:LYS:NZ	2.47	0.54
5:B:78:U:OP1	26:W:28:ARG:NH2	2.41	0.54
3:4:136:VAL:O	3:4:137:LYS:HB2	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:163:GLN:HB3	3:4:314:ALA:HB3	1.90	0.53
15:L:90:ASP:OD2	15:L:90:ASP:N	2.40	0.53
3:4:339:PRO:CG	3:4:382:LEU:HD21	2.38	0.53
3:4:420:VAL:HG23	3:4:466:TYR:CA	2.38	0.53
3:4:463:LEU:HD12	3:4:463:LEU:H	1.73	0.53
4:A:708:G:N2	8:E:187:ASP:OD1	2.41	0.53
3:4:246:PRO:HD3	3:4:293:ARG:HB3	1.90	0.53
3:4:463:LEU:CD1	3:4:463:LEU:H	2.22	0.53
4:A:2219:U:OP1	7:D:133:ARG:NH2	2.42	0.53
20:Q:62:LYS:HE2	20:Q:64:SER:HB3	1.90	0.53
3:4:173:LEU:HB3	3:4:174:PRO:HD3	1.90	0.53
27:X:11:ARG:O	27:X:14:ARG:NH1	2.38	0.53
3:4:263:ASN:HD21	3:4:270:VAL:N	2.04	0.53
3:4:426:ARG:HG2	3:4:427:GLY:N	2.24	0.53
4:A:571:A:OP1	4:A:572:C:N4	2.34	0.53
4:A:1535:C:H3'	4:A:1536:A:H8	1.73	0.53
11:H:98:ALA:O	11:H:102:ASN:ND2	2.41	0.53
26:W:186:SER:OG	26:W:187:ALA:N	2.41	0.53
3:4:214:ARG:O	3:4:218:ARG:HD3	2.09	0.53
5:B:48:C:OP2	19:P:14:ARG:NH1	2.42	0.53
8:E:119:ALA:HB2	8:E:124:ILE:HD12	1.90	0.53
9:F:103:MET:HG3	9:F:107:LEU:HD12	1.91	0.53
19:P:50:GLN:CA	19:P:63:ALA:HB3	2.37	0.53
3:4:87:GLN:HE21	4:A:2133:G:H8	1.55	0.53
3:4:377:VAL:C	3:4:379:LEU:H	2.12	0.53
4:A:1436:C:O2'	23:T:18:ARG:NH2	2.42	0.53
4:A:2536:U:O2	9:F:44:ASN:ND2	2.42	0.53
3:4:280:LEU:HD12	3:4:315:PHE:CZ	2.44	0.53
3:4:368:VAL:HB	3:4:371:ILE:HD11	1.91	0.53
3:4:136:VAL:HG23	3:4:138:VAL:H	1.73	0.52
3:4:202:GLY:N	3:4:203:PRO:CD	2.72	0.52
4:A:2380:G:N2	4:A:2382:G:OP2	2.43	0.52
4:A:1113:C:O2	14:K:3:THR:OG1	2.25	0.52
11:H:77:ASP:HB2	11:H:147:ASN:HB2	1.90	0.52
4:A:1337:G:OP2	22:S:91:ARG:NH1	2.42	0.52
3:4:213:ARG:HB3	3:4:214:ARG:HH21	1.74	0.52
3:4:365:LEU:HD11	3:4:388:ASP:CB	2.40	0.52
3:4:416:ALA:O	3:4:454:ARG:HB2	2.08	0.52
4:A:2519:C:OP2	19:P:24:ARG:NH2	2.43	0.52
15:L:47:ILE:HG22	15:L:49:GLY:H	1.74	0.52
3:4:73:LEU:HG	3:4:146:LEU:CD2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:73:LEU:HG	3:4:146:LEU:HG	1.91	0.52
3:4:369:ASN:C	3:4:371:ILE:H	2.13	0.52
19:P:41:ASN:ND2	19:P:48:HIS:O	2.43	0.52
13:J:125:ALA:O	13:J:129:ILE:HB	2.09	0.52
3:4:215:ILE:O	3:4:219:MET:HG3	2.10	0.52
3:4:85:LEU:HD13	3:4:106:LEU:HD21	1.89	0.52
3:4:330:HIS:NE2	3:4:346:VAL:HB	2.25	0.52
3:4:348:THR:O	3:4:351:ASN:HB2	2.10	0.52
4:A:349:G:H2'	4:A:350:A:H8	1.75	0.52
3:4:124:LEU:HD12	3:4:124:LEU:N	2.25	0.52
3:4:180:GLY:HA2	3:4:183:MET:HG2	1.91	0.52
3:4:328:LEU:HD12	3:4:328:LEU:N	2.24	0.52
3:4:432:ARG:NE	3:4:459:LEU:HD12	2.24	0.52
4:A:306:U:OP2	11:H:41:ARG:NH1	2.43	0.52
4:A:724:G:N2	4:A:727:A:OP2	2.36	0.52
3:4:132:LEU:HG	3:4:140:VAL:HG11	1.91	0.52
4:A:1076:A:N6	17:N:83:MET:HE1	2.24	0.52
7:D:144:VAL:HA	7:D:147:ARG:HG3	1.92	0.52
13:J:111:ALA:HB2	13:J:126:ALA:HB2	1.91	0.52
3:4:102:LYS:HD3	4:A:2133:G:P	2.50	0.51
3:4:227:ARG:HE	3:4:227:ARG:CA	2.20	0.51
13:J:21:ASN:ND2	13:J:41:CYS:SG	2.82	0.51
26:W:178:VAL:HG12	26:W:179:VAL:HG23	1.91	0.51
3:4:82:LEU:HD12	3:4:115:ALA:HB2	1.92	0.51
3:4:222:LEU:CD2	3:4:226:ILE:HG23	2.40	0.51
3:4:248:VAL:HG21	3:4:295:PHE:CD1	2.45	0.51
4:A:2726:G:H5''	4:A:2727:A:H5''	1.91	0.51
6:C:146:GLU:HB2	6:C:189:CYS:HB3	1.93	0.51
3:4:151:PHE:CE1	3:4:315:PHE:CE2	2.99	0.51
12:I:76:PRO:O	12:I:106:LYS:NZ	2.33	0.51
16:M:94:GLY:N	16:M:97:GLU:OE1	2.43	0.51
3:4:106:LEU:O	3:4:109:VAL:HG22	2.11	0.51
3:4:280:LEU:HD12	3:4:315:PHE:HZ	1.74	0.51
3:4:456:PRO:HB2	3:4:458:PRO:HD2	1.92	0.51
3:4:55:TRP:CG	3:4:55:TRP:O	2.64	0.51
3:4:119:ILE:N	3:4:119:ILE:HD12	2.24	0.51
4:A:2142:A:H2'	4:A:2143:A:O4'	2.10	0.51
25:V:10:LEU:HD13	25:V:80:PRO:HG3	1.92	0.51
3:4:48:ARG:HB2	3:4:116:ASP:OD1	2.11	0.51
3:4:335:SER:HB3	3:4:375:THR:OG1	2.11	0.51
3:4:420:VAL:HA	3:4:466:TYR:CD1	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:47:GLU:HA	3:4:79:SER:CB	2.40	0.51
3:4:49:VAL:HG22	3:4:81:VAL:HA	1.91	0.51
3:4:223:ARG:HA	3:4:226:ILE:CD1	2.41	0.51
4:A:1212:U:H4'	4:A:1215:U:H5	1.76	0.51
4:A:1546:A:N6	4:A:1625:G:O6	2.44	0.51
4:A:2983:G:N2	10:G:140:GLN:OE1	2.43	0.51
12:I:3:LYS:O	12:I:7:ALA:CB	2.59	0.51
3:4:180:GLY:CA	3:4:183:MET:HG2	2.40	0.51
4:A:2138:C:H4'	4:A:2142:A:C2	2.46	0.51
3:4:76:THR:O	3:4:76:THR:HG22	2.10	0.51
3:4:261:LEU:HD11	3:4:392:VAL:CG1	2.29	0.51
4:A:2476:G:H2'	4:A:2477:G:C8	2.45	0.51
3:4:70:LEU:HD22	3:4:121:ASP:HB3	1.92	0.50
3:4:178:GLY:C	3:4:180:GLY:H	2.14	0.50
3:4:392:VAL:HG13	3:4:400:LEU:HD23	1.92	0.50
4:A:1566:A:N6	4:A:1606:G:N2	2.47	0.50
3:4:430:VAL:HG12	3:4:434:HIS:HD2	1.75	0.50
3:4:456:PRO:HD2	3:4:459:LEU:HB2	1.94	0.50
3:4:148:LEU:HD11	3:4:168:GLN:HB3	1.92	0.50
3:4:436:ASP:HB3	3:4:439:VAL:CG2	2.41	0.50
3:4:458:PRO:HG2	3:4:459:LEU:HD22	1.93	0.50
13:J:48:THR:HB	13:J:56:ILE:HD13	1.94	0.50
4:A:2176:A:N3	4:A:2784:C:O2'	2.39	0.50
5:B:101:U:O3'	26:W:81:LYS:NZ	2.45	0.50
12:I:33:VAL:O	12:I:37:ALA:N	2.39	0.50
19:P:49:VAL:HG12	19:P:50:GLN:N	2.26	0.50
3:4:456:PRO:CB	3:4:459:LEU:HD23	2.38	0.50
4:A:2323:G:O6	4:A:2412:U:O4	2.30	0.50
4:A:2528:G:N2	9:F:160:ASP:OD2	2.45	0.50
3:4:46:LEU:HD22	3:4:46:LEU:N	2.26	0.50
3:4:95:SER:O	3:4:131:ALA:HB3	2.11	0.50
3:4:193:GLY:O	3:4:194:ALA:C	2.49	0.50
3:4:294:PRO:C	3:4:296:VAL:N	2.62	0.50
3:4:371:ILE:CA	3:4:374:ALA:HB2	2.35	0.50
3:4:420:VAL:CG2	3:4:421:THR:N	2.72	0.50
3:4:452:LYS:NZ	3:4:452:LYS:HB3	2.26	0.50
17:N:84:GLY:O	17:N:85:SER:OG	2.28	0.50
3:4:419:ASP:HA	3:4:452:LYS:HA	1.93	0.50
3:4:424:TYR:CE2	3:4:447:ALA:HA	2.47	0.50
4:A:1209:G:N2	4:A:1219:U:O2	2.40	0.50
4:A:2086:U:H3	4:A:2096:G:H1	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:84:ASN:HB2	16:M:118:LEU:HD12	1.94	0.50
3:4:89:ARG:HD3	3:4:91:LYS:O	2.11	0.49
3:4:284:THR:O	3:4:285:ARG:HD3	2.12	0.49
25:V:86:ARG:HB2	25:V:97:ILE:HD12	1.94	0.49
3:4:331:VAL:HA	3:4:367:VAL:O	2.12	0.49
3:4:392:VAL:HG13	3:4:400:LEU:HD21	1.94	0.49
7:D:14:THR:OG1	7:D:15:GLN:N	2.44	0.49
10:G:36:ASP:OD1	10:G:36:ASP:N	2.46	0.49
3:4:173:LEU:N	3:4:174:PRO:CD	2.75	0.49
3:4:187:ALA:C	3:4:189:GLY:H	2.15	0.49
4:A:2086:U:O4	4:A:2096:G:O6	2.30	0.49
3:4:201:ARG:NH2	4:A:2286:A:N7	2.60	0.49
4:A:1176:G:HO2'	4:A:1178:U:H3	1.59	0.49
3:4:110:VAL:HG21	3:4:138:VAL:HG21	1.94	0.49
3:4:222:LEU:HD23	3:4:226:ILE:HG23	1.95	0.49
3:4:382:LEU:O	3:4:386:LEU:HB2	2.13	0.49
8:E:184:ASN:OD1	8:E:184:ASN:N	2.45	0.49
12:I:77:THR:OG1	12:I:106:LYS:NZ	2.45	0.49
3:4:230:LYS:HD3	3:4:233:ARG:HH21	1.77	0.49
4:A:1209:G:N1	4:A:1219:U:C2	2.77	0.49
4:A:1548:C:H42	4:A:1621:C:H5	1.60	0.49
4:A:2400:C:H3'	4:A:2401:U:H4'	1.95	0.49
10:G:35:LEU:HD22	10:G:76:LEU:HD22	1.95	0.49
3:4:250:ILE:HD13	3:4:258:LYS:CA	2.40	0.49
3:4:350:ILE:O	3:4:354:VAL:HG23	2.12	0.49
3:4:432:ARG:O	3:4:433:VAL:C	2.51	0.49
19:P:43:SER:CB	19:P:47:ILE:HG22	2.41	0.49
3:4:166:LEU:HD22	3:4:226:ILE:CD1	2.43	0.49
4:A:920:G:N2	4:A:944:A:OP1	2.44	0.49
7:D:7:LEU:HB2	7:D:34:ASN:HD21	1.78	0.49
14:K:49:ASP:OD1	14:K:121:LYS:NZ	2.44	0.49
3:4:87:GLN:HG2	3:4:88:ARG:H	1.78	0.49
3:4:88:ARG:HG2	4:A:2137:A:N6	2.28	0.49
3:4:173:LEU:CD1	3:4:215:ILE:HG21	2.34	0.49
3:4:181:GLU:C	3:4:184:SER:H	2.16	0.49
4:A:347:U:H2'	4:A:348:G:C8	2.47	0.49
4:A:2137:A:H4'	4:A:2142:A:C2	2.47	0.49
4:A:2224:C:O2'	4:A:2913:U:OP2	2.30	0.49
27:X:53:ARG:NH1	27:X:57:ASP:OD1	2.46	0.49
3:4:125:SER:OG	3:4:128:GLN:HG3	2.13	0.49
3:4:158:ARG:HD2	3:4:158:ARG:C	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:233:ARG:O	3:4:237:ARG:HG2	2.13	0.49
4:A:2329:G:O6	4:A:2406:U:O4	2.30	0.49
3:4:288:GLU:HG2	3:4:289:PHE:O	2.13	0.48
3:4:295:PHE:O	3:4:295:PHE:CD1	2.66	0.48
4:A:1184:U:O5'	4:A:1187:A:N6	2.45	0.48
4:A:2161:A:O2'	4:A:2163:U:OP2	2.24	0.48
23:T:77:VAL:HG21	23:T:117:ARG:HD2	1.95	0.48
3:4:45:ARG:CZ	3:4:45:ARG:HB3	2.43	0.48
3:4:251:VAL:CG2	3:4:252:GLY:N	2.74	0.48
4:A:2141:U:O2'	4:A:2142:A:H5''	2.12	0.48
6:C:143:HIS:ND1	6:C:194:GLY:O	2.30	0.48
12:I:53:LYS:O	12:I:54:ASN:ND2	2.45	0.48
23:T:9:SER:HB3	23:T:115:GLU:HG2	1.94	0.48
3:4:199:GLY:O	3:4:201:ARG:N	2.47	0.48
3:4:213:ARG:CB	3:4:214:ARG:HH21	2.26	0.48
11:H:101:VAL:HG22	11:H:114:LYS:HB2	1.96	0.48
12:I:115:LEU:HD11	12:I:119:ASP:HB3	1.94	0.48
3:4:187:ALA:CB	4:A:2826:A:C5	2.97	0.48
3:4:223:ARG:O	3:4:226:ILE:HG12	2.13	0.48
3:4:395:ARG:HG2	3:4:396:THR:N	2.26	0.48
3:4:463:LEU:HD12	3:4:463:LEU:N	2.29	0.48
4:A:1163:A:OP1	4:A:1229:A:N6	2.46	0.48
4:A:2530:C:H3'	4:A:2531:G:H2'	1.94	0.48
22:S:27:LEU:HB2	22:S:95:THR:HG21	1.95	0.48
3:4:142:ASP:OD1	3:4:142:ASP:N	2.46	0.48
3:4:287:GLY:O	3:4:294:PRO:O	2.32	0.48
6:C:182:ILE:HB	6:C:269:VAL:HB	1.95	0.48
11:H:118:GLN:HE21	11:H:120:ALA:HB3	1.79	0.48
12:I:119:ASP:HA	12:I:122:LYS:HD2	1.95	0.48
19:P:79:ALA:HB3	19:P:115:ALA:HB3	1.95	0.48
3:4:185:ARG:C	3:4:187:ALA:H	2.17	0.48
3:4:397:GLY:O	3:4:398:ASP:C	2.50	0.48
4:A:1157:G:N2	4:A:1234:U:O2	2.47	0.48
4:A:1160:G:H1	4:A:1230:G:H22	1.61	0.48
11:H:85:ALA:N	11:H:90:LYS:O	2.46	0.48
4:A:356:G:H21	4:A:362:A:H62	1.62	0.48
4:A:1548:C:C2	4:A:1622:G:H1'	2.49	0.48
5:B:44:C:O3'	9:F:102:ARG:NH2	2.46	0.48
9:F:45:MET:HG3	9:F:64:LEU:HD22	1.95	0.48
3:4:102:LYS:CG	4:A:2132:U:H5'	2.31	0.48
3:4:151:PHE:HE2	3:4:277:PHE:CG	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:329:ILE:HA	3:4:365:LEU:O	2.14	0.48
3:4:395:ARG:NH2	36:4:501:GCP:C2	2.62	0.48
4:A:2463:G:OP1	6:C:244:ARG:NH2	2.43	0.48
15:L:122:LEU:HD13	20:Q:69:VAL:HG11	1.95	0.48
3:4:49:VAL:CG2	3:4:81:VAL:HA	2.43	0.48
3:4:90:ASP:HB3	4:A:2137:A:C2	2.48	0.48
3:4:147:ILE:CD1	3:4:151:PHE:CE2	2.95	0.48
4:A:81:A:OP1	25:V:4:HIS:NE2	2.47	0.48
19:P:64:SER:OG	19:P:65:SER:N	2.47	0.48
3:4:76:THR:HG22	3:4:150:ILE:HD11	1.96	0.48
11:H:1:MET:N	11:H:21:VAL:O	2.44	0.48
11:H:100:VAL:HG23	11:H:114:LYS:HG3	1.96	0.48
26:W:50:ASN:ND2	26:W:53:ASP:OD1	2.41	0.48
4:A:1537:U:H2'	4:A:1538:G:H8	1.78	0.47
4:A:1542:A:N1	4:A:1628:A:O2'	2.41	0.47
10:G:17:VAL:HG12	10:G:26:VAL:HG22	1.96	0.47
11:H:75:LEU:O	11:H:145:SER:OG	2.31	0.47
4:A:1116:C:OP2	21:R:58:ARG:NH2	2.47	0.47
4:A:1200:U:HO2'	12:I:50:THR:HG1	1.60	0.47
4:A:3014:A:H62	4:A:3113:A:H2	1.62	0.47
24:U:30:THR:HG23	24:U:83:ILE:HG12	1.96	0.47
12:I:45:ASP:OD2	12:I:45:ASP:N	2.46	0.47
20:Q:91:VAL:HG11	20:Q:96:LEU:HD21	1.95	0.47
3:4:436:ASP:CB	3:4:439:VAL:CG1	2.92	0.47
17:N:43:THR:OG1	17:N:44:ASN:N	2.41	0.47
3:4:151:PHE:CE1	3:4:315:PHE:CZ	3.03	0.47
3:4:426:ARG:NH2	3:4:433:VAL:HG11	2.30	0.47
3:4:455:VAL:CB	3:4:460:ALA:HB3	2.44	0.47
4:A:164:A:OP2	11:H:118:GLN:NE2	2.47	0.47
4:A:2367:G:N2	4:A:2370:A:C4	2.83	0.47
6:C:181:GLU:HG2	6:C:271:ARG:HA	1.96	0.47
13:J:12:LYS:HE2	13:J:59:GLU:HB2	1.97	0.47
21:R:26:GLY:O	21:R:30:ARG:NH1	2.48	0.47
3:4:231:LYS:O	3:4:235:THR:HG22	2.15	0.47
4:A:1198:C:H2'	13:J:128:LYS:HD2	1.96	0.47
4:A:2137:A:HO2'	4:A:2138:C:P	2.37	0.47
13:J:103:THR:OG1	13:J:104:TRP:N	2.46	0.47
3:4:258:LYS:HD3	36:4:501:GCP:O1B	2.15	0.47
3:4:432:ARG:HG2	3:4:459:LEU:HD12	1.95	0.47
4:A:551:G:N2	4:A:554:A:OP2	2.42	0.47
4:A:808:A:O2'	4:A:1468:A:N3	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2764:C:O2'	4:A:2964:A:N3	2.42	0.47
22:S:21:VAL:HG22	22:S:98:LYS:HG3	1.96	0.47
3:4:102:LYS:N	4:A:2132:U:OP1	2.41	0.47
4:A:994:A:N6	4:A:1014:G:O2'	2.46	0.47
4:A:2340:A:O2'	4:A:2342:A:OP1	2.32	0.47
9:F:124:LEU:HG	9:F:184:PHE:HA	1.96	0.47
10:G:99:LEU:HG	10:G:101:GLY:H	1.80	0.47
3:4:449:THR:OG1	3:4:451:ILE:HG12	2.15	0.47
4:A:1198:C:N4	4:A:1206:A:OP2	2.48	0.47
4:A:2371:G:O2'	4:A:2372:U:O4'	2.29	0.47
4:A:1365:G:O6	16:M:21:ARG:NH2	2.46	0.46
3:4:208:ILE:HG23	3:4:209:GLU:N	2.30	0.46
3:4:395:ARG:CG	3:4:396:THR:H	2.23	0.46
4:A:678:A:H5'	8:E:90:VAL:HG13	1.95	0.46
4:A:2367:G:C2	4:A:2370:A:C8	3.03	0.46
21:R:125:SER:O	21:R:125:SER:OG	2.32	0.46
3:4:433:VAL:O	3:4:439:VAL:HB	2.15	0.46
4:A:32:G:H1'	4:A:542:A:C4	2.50	0.46
4:A:1162:G:OP2	4:A:1164:A:N6	2.40	0.46
4:A:2136:A:N6	4:A:2139:U:O4	2.48	0.46
4:A:2385:G:H5''	4:A:2396:A:H61	1.80	0.46
10:G:51:ILE:HD12	10:G:70:ARG:HA	1.96	0.46
23:T:52:GLU:HG2	23:T:53:PRO:HD3	1.97	0.46
25:V:43:LYS:O	25:V:43:LYS:NZ	2.36	0.46
3:4:46:LEU:HA	3:4:116:ASP:OD2	2.15	0.46
4:A:256:A:H2'	4:A:257:A:H8	1.80	0.46
4:A:544:U:O2	4:A:547:U:O2'	2.26	0.46
19:P:49:VAL:O	19:P:50:GLN:HB3	2.15	0.46
19:P:49:VAL:O	19:P:64:SER:HA	2.16	0.46
19:P:68:ALA:O	19:P:71:ARG:NH1	2.49	0.46
3:4:253:TYR:CE1	3:4:332:VAL:HG12	2.37	0.46
4:A:1364:U:C4	16:M:21:ARG:HD3	2.51	0.46
18:O:106:ASP:OD2	18:O:106:ASP:N	2.48	0.46
19:P:52:VAL:HG13	19:P:59:THR:HG22	1.97	0.46
4:A:1269:C:O2'	21:R:121:VAL:O	2.29	0.46
4:A:1562:C:H2'	4:A:1563:A:H8	1.80	0.46
20:Q:48:ARG:HB2	20:Q:95:LYS:HD3	1.97	0.46
21:R:73:ASP:O	21:R:114:ARG:NH2	2.49	0.46
25:V:27:TYR:HB2	25:V:30:ARG:HB2	1.98	0.46
27:X:76:LYS:HB3	27:X:76:LYS:HE3	1.72	0.46
28:Y:21:SER:O	28:Y:21:SER:OG	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:163:GLN:HB3	3:4:314:ALA:CB	2.45	0.46
3:4:232:ILE:HA	3:4:235:THR:HG22	1.97	0.46
3:4:438:HIS:CE1	3:4:456:PRO:HG3	2.51	0.46
4:A:1577:C:H2'	4:A:1578:G:H8	1.81	0.46
4:A:2527:G:O2'	9:F:128:GLN:O	2.33	0.46
7:D:10:LYS:HB3	7:D:198:ILE:HD11	1.98	0.46
10:G:19:ILE:HG12	10:G:24:LEU:HD13	1.97	0.46
19:P:62:ALA:HB3	19:P:91:ARG:HH12	1.81	0.46
3:4:147:ILE:O	3:4:147:ILE:HD12	2.15	0.46
3:4:240:ARG:HG2	4:A:2697:U:O2	2.16	0.46
3:4:393:SER:O	36:4:501:GCP:O6	2.34	0.46
11:H:74:GLY:HA3	11:H:105:LYS:HE3	1.96	0.46
3:4:172:MET:O	3:4:172:MET:SD	2.74	0.46
9:F:132:THR:HG22	9:F:170:ASP:HA	1.98	0.46
3:4:361:PRO:HA	3:4:362:PRO:HD3	1.84	0.46
3:4:430:VAL:HG12	3:4:434:HIS:CD2	2.51	0.46
3:4:445:THR:OG1	3:4:449:THR:HA	2.16	0.46
4:A:531:A:H2'	8:E:46:ARG:HH12	1.81	0.45
4:A:2008:A:N6	4:A:2045:G:O2'	2.42	0.45
13:J:106:GLN:HB3	13:J:109:GLU:HB3	1.97	0.45
25:V:44:HIS:H	25:V:59:ILE:HG12	1.80	0.45
3:4:289:PHE:HD1	3:4:290:GLU:H	1.64	0.45
3:4:332:VAL:HG11	3:4:343:ILE:HG12	1.97	0.45
4:A:1209:G:C6	4:A:1219:U:N3	2.84	0.45
5:B:9:G:O6	5:B:109:C:N4	2.49	0.45
12:I:20:SER:HA	12:I:83:LYS:HD3	1.99	0.45
19:P:67:GLU:OE2	19:P:91:ARG:NH1	2.49	0.45
2:3:16:ALA:O	4:A:1096:G:N2	2.37	0.45
3:4:201:ARG:HG3	4:A:2675:A:H2	1.80	0.45
3:4:426:ARG:HG3	3:4:429:LEU:CB	2.28	0.45
4:A:1705:C:H2'	4:A:1706:A:H8	1.80	0.45
12:I:82:VAL:HG11	12:I:90:ALA:HB2	1.97	0.45
19:P:39:VAL:O	19:P:49:VAL:CG1	2.64	0.45
3:4:89:ARG:HG2	3:4:91:LYS:H	1.81	0.45
3:4:370:LYS:HD3	36:4:501:GCP:C4	2.45	0.45
3:4:460:ALA:O	3:4:463:LEU:HD13	2.16	0.45
14:K:28:LEU:HD22	14:K:62:ILE:HD11	1.98	0.45
3:4:48:ARG:HD2	3:4:82:LEU:HD11	1.98	0.45
3:4:102:LYS:HG2	4:A:2132:U:OP1	2.16	0.45
3:4:301:VAL:HG12	3:4:302:GLY:N	2.32	0.45
2:3:7:LYS:NZ	4:A:1252:G:OP2	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:125:SER:HB2	3:4:126:PRO:CD	2.47	0.45
3:4:305:ARG:HG2	3:4:306:HIS:CD2	2.52	0.45
3:4:430:VAL:O	3:4:433:VAL:N	2.50	0.45
22:S:8:LYS:HG2	22:S:13:GLN:HG2	1.99	0.45
4:A:2137:A:O4'	4:A:2143:A:N6	2.50	0.45
4:A:2323:G:C6	4:A:2412:U:N3	2.84	0.45
19:P:47:ILE:HG21	19:P:112:ARG:HD3	1.99	0.45
3:4:151:PHE:CD1	3:4:311:LEU:HD12	2.52	0.45
3:4:327:LEU:HD21	3:4:329:ILE:HD13	1.98	0.45
3:4:391:PHE:CD1	3:4:391:PHE:N	2.83	0.45
4:A:380:A:N3	4:A:401:C:O2'	2.41	0.45
6:C:240:THR:OG1	6:C:241:SER:N	2.50	0.45
3:4:317:SER:O	3:4:321:GLU:HG2	2.16	0.45
4:A:368:U:H3	4:A:434:G:H1	1.64	0.45
4:A:1194:C:C2	13:J:93:GLU:HG2	2.52	0.45
4:A:1198:C:C2	13:J:128:LYS:HE3	2.52	0.45
4:A:1582:C:N4	4:A:1583:U:O2	2.50	0.45
4:A:2321:U:O4	4:A:2414:G:O6	2.35	0.45
9:F:76:ARG:HD3	9:F:89:GLY:HA2	1.99	0.45
19:P:26:ARG:NH2	19:P:54:ASP:OD2	2.38	0.45
21:R:68:ALA:O	21:R:72:ASN:ND2	2.48	0.45
3:4:89:ARG:CD	3:4:92:PRO:HA	2.47	0.45
3:4:93:ASP:OD2	3:4:94:PRO:HD2	2.17	0.45
3:4:416:ALA:HB1	3:4:455:VAL:N	2.32	0.45
9:F:110:LEU:HA	9:F:114:ALA:HB3	1.99	0.45
13:J:102:VAL:HB	13:J:141:VAL:HG13	1.99	0.45
25:V:45:THR:OG1	25:V:46:ALA:N	2.49	0.45
3:4:199:GLY:C	3:4:201:ARG:HD2	2.37	0.44
3:4:323:VAL:HG11	3:4:357:TYR:HD1	1.82	0.44
4:A:2348:G:N2	4:A:2394:A:OP2	2.49	0.44
4:A:3012:U:O2'	4:A:3030:A:N3	2.42	0.44
13:J:105:ASP:OD1	13:J:105:ASP:N	2.45	0.44
3:4:167:ALA:HA	3:4:170:GLU:OE2	2.18	0.44
3:4:271:LEU:HD21	3:4:273:GLU:CB	2.45	0.44
4:A:858:A:O2'	4:A:1877:U:OP1	2.35	0.44
4:A:1022:C:O2'	17:N:101:ARG:NH2	2.49	0.44
5:B:112:C:C4	5:B:113:G:H1'	2.53	0.44
8:E:47:GLN:HE21	8:E:47:GLN:HB3	1.61	0.44
25:V:77:ASP:OD1	25:V:101:ASN:ND2	2.50	0.44
27:X:72:LYS:HD3	27:X:72:LYS:HA	1.70	0.44
3:4:254:THR:OG1	36:4:501:GCP:O1G	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:440:ASP:O	3:4:441:ALA:HB3	2.17	0.44
4:A:1179:U:C2	13:J:11:ILE:HD11	2.53	0.44
12:I:40:ARG:HD2	13:J:123:ILE:HD13	1.99	0.44
3:4:326:ASP:CB	3:4:412:GLU:OE1	2.57	0.44
4:A:576:G:O2'	23:T:56:LYS:NZ	2.34	0.44
4:A:718:C:O2'	4:A:772:U:OP1	2.31	0.44
10:G:27:LYS:HA	10:G:32:THR:HG22	1.98	0.44
11:H:30:LEU:HD13	11:H:35:LEU:HB2	1.98	0.44
12:I:3:LYS:HG3	12:I:7:ALA:HB2	1.98	0.44
13:J:128:LYS:HD2	13:J:128:LYS:HA	1.71	0.44
22:S:69:LYS:HD2	22:S:91:ARG:HG2	2.00	0.44
3:4:186:GLN:HG3	3:4:207:LYS:HZ1	1.83	0.44
3:4:383:ARG:NE	3:4:391:PHE:CZ	2.85	0.44
4:A:279:U:H2'	4:A:280:G:H8	1.83	0.44
4:A:499:G:OP2	4:A:2630:A:O2'	2.33	0.44
5:B:15:U:OP2	5:B:71:C:O2'	2.34	0.44
6:C:85:ASP:OD2	6:C:88:ARG:NH1	2.47	0.44
12:I:6:LYS:HE2	12:I:6:LYS:HB3	1.82	0.44
3:4:383:ARG:HH11	3:4:383:ARG:CB	2.31	0.44
3:4:441:ALA:H	3:4:453:ALA:HB2	1.82	0.44
4:A:1249:G:H4'	14:K:84:LEU:HD22	1.99	0.44
4:A:1314:C:H1'	21:R:4:VAL:HG12	1.99	0.44
5:B:8:C:H2'	5:B:9:G:H4'	1.98	0.44
10:G:20:ASN:OD1	10:G:20:ASN:N	2.50	0.44
19:P:126:LYS:HE2	19:P:126:LYS:HB3	1.80	0.44
3:4:305:ARG:NH1	3:4:345:ALA:HB2	2.32	0.44
3:4:393:SER:O	3:4:394:ALA:HB3	2.17	0.44
4:A:1210:C:H3'	4:A:1211:G:C8	2.52	0.44
4:A:1541:G:HO2'	4:A:1632:G:N2	2.16	0.44
10:G:28:GLY:HA2	10:G:80:VAL:HG22	1.99	0.44
3:4:96:THR:O	3:4:98:ILE:N	2.49	0.44
3:4:165:SER:HA	3:4:168:GLN:CG	2.48	0.44
3:4:193:GLY:CA	4:A:2809:U:H1'	2.48	0.44
3:4:367:VAL:HG22	3:4:388:ASP:OD2	2.18	0.44
3:4:393:SER:C	3:4:395:ARG:N	2.71	0.44
12:I:43:LEU:HB3	12:I:92:ALA:HB1	1.99	0.44
19:P:49:VAL:O	19:P:64:SER:CA	2.66	0.44
3:4:243:SER:O	3:4:245:ILE:HG23	2.18	0.44
3:4:248:VAL:HG23	3:4:297:LEU:HD13	2.00	0.44
3:4:371:ILE:O	3:4:373:ALA:N	2.51	0.44
4:A:998:G:H1	4:A:1009:U:H3	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1708:A:H1'	4:A:1709:U:H5'	2.00	0.44
17:N:10:ARG:HG2	17:N:90:PRO:HG2	2.00	0.44
3:4:50:VAL:HG23	3:4:50:VAL:O	2.18	0.43
3:4:204:GLY:O	3:4:205:GLU:HG3	2.17	0.43
3:4:456:PRO:HG2	3:4:459:LEU:HD23	1.98	0.43
4:A:1185:A:OP1	4:A:1187:A:N6	2.50	0.43
4:A:1537:U:H2'	4:A:1538:G:C8	2.53	0.43
9:F:178:ARG:NH2	9:F:186:GLU:OE2	2.48	0.43
3:4:300:THR:CB	3:4:318:THR:HG23	2.44	0.43
3:4:369:ASN:OD1	3:4:370:LYS:HG2	2.17	0.43
4:A:1302:G:N2	4:A:1303:U:O4	2.48	0.43
4:A:2143:A:N6	4:A:2144:C:N4	2.66	0.43
4:A:2249:G:H2'	4:A:2250:A:C8	2.54	0.43
11:H:83:ASN:HB3	11:H:92:PHE:HB2	2.01	0.43
19:P:37:ARG:NE	19:P:54:ASP:OD2	2.51	0.43
23:T:11:THR:HG22	23:T:113:ILE:HG12	2.01	0.43
3:4:230:LYS:HE2	3:4:234:ASP:OD1	2.18	0.43
3:4:272:VAL:CG2	36:4:501:GCP:H5'2	2.48	0.43
3:4:327:LEU:HD12	3:4:410:LEU:HB2	2.00	0.43
3:4:381:GLN:HG2	3:4:384:ARG:HD3	2.00	0.43
3:4:426:ARG:O	3:4:428:ASP:N	2.51	0.43
3:4:432:ARG:HB3	3:4:436:ASP:CG	2.38	0.43
3:4:443:GLU:CD	3:4:452:LYS:HD3	2.39	0.43
4:A:1210:C:H3'	4:A:1211:G:H8	1.84	0.43
4:A:2070:A:H2'	4:A:2071:A:C8	2.53	0.43
5:B:9:G:N1	5:B:109:C:N3	2.66	0.43
6:C:37:LEU:HG	6:C:62:TYR:HB2	1.98	0.43
9:F:9:PRO:HG3	9:F:104:TRP:HA	2.00	0.43
12:I:31:LEU:HD13	12:I:36:LEU:HD21	1.98	0.43
12:I:94:LYS:HE2	12:I:105:ILE:HD13	1.99	0.43
12:I:95:LYS:HA	12:I:95:LYS:HD3	1.82	0.43
15:L:80:ASP:OD2	20:Q:103:ARG:NH1	2.51	0.43
3:4:167:ALA:HA	3:4:170:GLU:HG2	2.00	0.43
3:4:195:GLY:C	3:4:197:GLY:N	2.69	0.43
3:4:328:LEU:CD1	3:4:362:PRO:HB2	2.48	0.43
3:4:272:VAL:O	3:4:272:VAL:HG22	2.18	0.43
4:A:114:G:OP2	4:A:116:A:O2'	2.29	0.43
4:A:738:A:H4'	4:A:739:U:H5	1.82	0.43
4:A:1207:G:N7	13:J:118:LEU:HG	2.33	0.43
4:A:2143:A:C6	4:A:2144:C:C4	3.06	0.43
17:N:51:ARG:HD3	17:N:66:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:87:GLN:NE2	4:A:2133:G:C8	2.77	0.43
3:4:110:VAL:HG21	3:4:138:VAL:CG2	2.48	0.43
3:4:348:THR:HA	3:4:351:ASN:ND2	2.33	0.43
3:4:393:SER:O	3:4:395:ARG:N	2.44	0.43
4:A:325:U:C2	4:A:450:G:N1	2.86	0.43
4:A:1558:C:H2'	4:A:1559:A:C8	2.53	0.43
11:H:86:GLY:HA3	11:H:90:LYS:HB3	2.00	0.43
3:4:357:TYR:N	3:4:357:TYR:CD2	2.86	0.43
3:4:371:ILE:CG2	3:4:372:ASP:N	2.80	0.43
3:4:436:ASP:CB	3:4:439:VAL:HG22	2.49	0.43
3:4:441:ALA:H	3:4:453:ALA:HB1	1.83	0.43
4:A:2735:U:O2'	7:D:148:PRO:O	2.29	0.43
26:W:124:VAL:HG22	26:W:181:VAL:HG22	2.00	0.43
3:4:105:GLU:OE1	3:4:105:GLU:HA	2.18	0.43
3:4:420:VAL:CG2	3:4:421:THR:H	2.25	0.43
4:A:314:G:O2'	4:A:321:G:O2'	2.36	0.43
4:A:546:G:O2'	4:A:557:G:O6	2.32	0.43
4:A:2017:C:OP2	6:C:183:ARG:NH2	2.40	0.43
8:E:13:LYS:HB3	8:E:13:LYS:HE3	1.88	0.43
10:G:164:ARG:HG3	10:G:165:TYR:H	1.84	0.43
26:W:50:ASN:O	26:W:54:PHE:HB2	2.19	0.43
3:4:228:ASP:C	3:4:230:LYS:N	2.70	0.43
3:4:254:THR:O	3:4:255:ASN:HB2	2.19	0.43
3:4:289:PHE:CD2	3:4:404:ARG:HG2	2.54	0.43
4:A:1172:A:H62	4:A:1203:A:N6	2.17	0.43
4:A:2138:C:N4	4:A:2141:U:O4	2.52	0.43
8:E:183:LEU:HD23	8:E:183:LEU:HA	1.87	0.43
19:P:76:ASP:HB3	19:P:80:HIS:HA	2.01	0.43
3:4:85:LEU:HD21	3:4:106:LEU:CD2	2.49	0.43
3:4:316:ARG:O	3:4:320:GLU:HG3	2.18	0.43
3:4:426:ARG:CG	3:4:427:GLY:N	2.81	0.43
5:B:81:U:H2'	5:B:82:A:C8	2.53	0.43
10:G:46:ALA:HB3	10:G:50:ALA:HB3	2.00	0.43
19:P:41:ASN:N	19:P:49:VAL:HG22	2.34	0.43
3:4:46:LEU:O	3:4:47:GLU:CB	2.65	0.42
3:4:295:PHE:CE1	3:4:407:MET:SD	3.13	0.42
4:A:21:G:O2'	23:T:85:GLU:O	2.31	0.42
4:A:1668:C:O2'	4:A:1764:A:N3	2.42	0.42
12:I:115:LEU:HD21	12:I:123:ILE:HD12	2.01	0.42
3:4:305:ARG:HH22	3:4:341:ALA:C	2.22	0.42
3:4:435:THR:HG23	3:4:435:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2552:A:H2'	4:A:2553:G:C8	2.54	0.42
4:A:2970:U:H4'	10:G:139:LYS:HB2	2.02	0.42
3:4:82:LEU:CD1	3:4:113:THR:HB	2.40	0.42
4:A:759:G:N1	27:X:64:PRO:HB3	2.34	0.42
4:A:2083:A:N6	4:A:2099:G:O2'	2.51	0.42
4:A:2135:U:C5	4:A:2137:A:H8	2.37	0.42
4:A:2323:G:N1	4:A:2412:U:N3	2.68	0.42
4:A:2340:A:N6	4:A:2388:G:O6	2.44	0.42
4:A:2515:U:H2'	4:A:2516:U:C6	2.53	0.42
8:E:2:THR:OG1	8:E:20:LEU:O	2.37	0.42
22:S:80:ASN:OD1	22:S:80:ASN:N	2.51	0.42
27:X:50:ASN:HD22	27:X:50:ASN:HA	1.67	0.42
3:4:357:TYR:N	3:4:357:TYR:HD2	2.17	0.42
3:4:426:ARG:HE	3:4:430:VAL:CG1	2.25	0.42
3:4:434:HIS:CB	4:A:1185:A:H1'	2.37	0.42
4:A:2116:C:H2'	4:A:2117:C:H6	1.84	0.42
4:A:2529:A:H2'	4:A:2530:C:C6	2.54	0.42
3:4:133:GLU:O	3:4:137:LYS:HA	2.19	0.42
3:4:199:GLY:CA	3:4:201:ARG:CZ	2.97	0.42
4:A:2973:A:H4'	10:G:63:ARG:HG2	2.01	0.42
9:F:56:LEU:HD13	9:F:56:LEU:HA	1.88	0.42
11:H:77:ASP:N	11:H:77:ASP:OD1	2.52	0.42
11:H:100:VAL:HG12	11:H:119:LEU:HD12	2.01	0.42
19:P:44:ALA:O	19:P:112:ARG:NH1	2.52	0.42
19:P:79:ALA:O	19:P:81:SER:N	2.53	0.42
3:4:118:VAL:C	3:4:119:ILE:HD12	2.39	0.42
3:4:124:LEU:HD13	3:4:142:ASP:HB3	2.00	0.42
3:4:443:GLU:CB	3:4:452:LYS:HB2	2.50	0.42
4:A:1690:A:H2'	4:A:1691:A:C8	2.54	0.42
4:A:2527:G:H2'	4:A:2528:G:C8	2.55	0.42
4:A:2753:G:H5''	4:A:2754:G:H5''	2.02	0.42
9:F:23:LEU:HD21	9:F:172:GLU:HG3	2.01	0.42
3:4:187:ALA:C	3:4:189:GLY:N	2.71	0.42
3:4:245:ILE:HG21	3:4:294:PRO:HG2	1.99	0.42
3:4:250:ILE:HG23	3:4:250:ILE:O	2.19	0.42
4:A:1212:U:H2'	4:A:1213:A:H5''	2.01	0.42
4:A:1479:G:H4'	4:A:2025:C:H5	1.85	0.42
18:O:38:GLU:OE1	18:O:42:ARG:NH2	2.47	0.42
3:4:55:TRP:O	3:4:55:TRP:CD1	2.73	0.42
4:A:928:U:H2'	4:A:929:C:C6	2.54	0.42
4:A:1621:C:H2'	4:A:1622:G:H4'	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1728:U:H4'	4:A:1729:A:H5'	2.02	0.42
19:P:111:GLY:H	19:P:114:ALA:HB3	1.85	0.42
3:4:143:ARG:NH2	3:4:305:ARG:O	2.51	0.42
4:A:1179:U:H2'	13:J:13:LEU:HA	2.01	0.42
4:A:1619:U:H2'	4:A:1620:U:C2	2.55	0.42
6:C:40:LYS:HB3	6:C:40:LYS:HE3	4.70	0.42
9:F:87:ARG:H	9:F:90:MET:HE1	1.84	0.42
16:M:104:VAL:HG11	16:M:110:VAL:HG13	2.02	0.42
3:4:93:ASP:HA	3:4:94:PRO:HD3	1.91	0.42
3:4:246:PRO:HA	3:4:326:ASP:OD2	2.20	0.42
3:4:283:THR:CG2	3:4:299:ASP:HB3	2.49	0.42
3:4:291:ASP:OD2	3:4:293:ARG:HG3	2.20	0.42
4:A:389:G:H21	4:A:412:A:H61	1.65	0.42
4:A:857:U:H2'	4:A:858:A:C8	2.54	0.42
4:A:960:G:OP2	4:A:960:G:N2	2.47	0.42
6:C:222:ARG:HE	6:C:222:ARG:HB2	1.67	0.42
6:C:258:ARG:NH2	6:C:264:SER:OG	2.53	0.42
12:I:33:VAL:HG21	13:J:117:ASP:HB2	2.02	0.42
3:4:184:SER:O	3:4:185:ARG:HB2	2.20	0.41
3:4:445:THR:HG23	3:4:450:ARG:H	1.84	0.41
6:C:163:ILE:HD12	6:C:175:LEU:HB3	2.01	0.41
11:H:119:LEU:HA	11:H:132:VAL:HG21	2.01	0.41
12:I:101:LYS:HD2	12:I:101:LYS:HA	1.78	0.41
26:W:86:HIS:CD2	26:W:87:PRO:HD2	2.55	0.41
3:4:410:LEU:HD12	3:4:410:LEU:N	2.34	0.41
4:A:1000:C:O2	4:A:1008:G:N1	2.53	0.41
5:B:9:G:H2'	5:B:10:G:C4	2.54	0.41
3:4:56:THR:HG23	3:4:57:GLU:OE2	2.21	0.41
3:4:319:LEU:HD12	3:4:319:LEU:N	2.35	0.41
3:4:424:TYR:CD1	3:4:424:TYR:N	2.88	0.41
4:A:1008:G:H2'	4:A:1009:U:C6	2.55	0.41
5:B:9:G:H5'	5:B:10:G:C8	2.56	0.41
6:C:132:PRO:HA	6:C:190:ARG:HA	2.01	0.41
6:C:147:LEU:HD23	6:C:147:LEU:HA	1.92	0.41
14:K:2:PRO:HB2	14:K:3:THR:H	1.60	0.41
19:P:56:ASN:OD1	19:P:56:ASN:N	2.51	0.41
25:V:40:ARG:HD3	25:V:61:THR:HG22	2.02	0.41
26:W:177:LEU:HD23	26:W:180:ASN:HB3	2.02	0.41
29:Z:11:ARG:O	29:Z:64:ARG:NH2	2.53	0.41
1:2:40:ASN:OD1	1:2:40:ASN:N	2.52	0.41
3:4:100:SER:HG	4:A:2131:G:H4'	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:357:TYR:O	3:4:358:ASP:C	2.59	0.41
4:A:264:G:H4'	4:A:516:G:H22	1.85	0.41
8:E:9:THR:HG22	8:E:128:THR:HG21	2.02	0.41
8:E:152:LYS:HG3	8:E:153:LYS:HG2	2.02	0.41
12:I:26:THR:H	12:I:78:ALA:HB3	1.86	0.41
19:P:87:LEU:HD23	19:P:87:LEU:HA	1.86	0.41
3:4:187:ALA:HB2	4:A:2826:A:N7	2.35	0.41
3:4:327:LEU:HD21	3:4:329:ILE:HD11	2.02	0.41
3:4:372:ASP:N	3:4:374:ALA:H	2.18	0.41
3:4:386:LEU:HD23	3:4:386:LEU:HA	1.76	0.41
4:A:1089:C:O2'	4:A:1101:A:N3	2.46	0.41
3:4:386:LEU:HA	3:4:387:PRO:HD3	1.89	0.41
3:4:429:LEU:HD13	3:4:429:LEU:HA	1.70	0.41
5:B:9:G:H2'	5:B:10:G:N9	2.36	0.41
6:C:79:VAL:HG22	6:C:115:ASP:H	1.86	0.41
7:D:125:GLY:O	7:D:129:ARG:HB3	2.20	0.41
3:4:284:THR:HG22	3:4:298:THR:HG23	2.02	0.41
3:4:308:PRO:HG2	3:4:311:LEU:HD21	2.01	0.41
5:B:27:A:N3	5:B:115:A:O2'	2.53	0.41
8:E:42:LEU:HD23	8:E:42:LEU:HA	1.94	0.41
9:F:110:LEU:HD23	9:F:114:ALA:HB3	2.03	0.41
10:G:27:LYS:NZ	10:G:28:GLY:O	2.47	0.41
12:I:3:LYS:HE3	12:I:59:ARG:HH11	1.85	0.41
3:4:186:GLN:CB	3:4:207:LYS:NZ	2.83	0.41
3:4:198:VAL:O	4:A:2286:A:N6	2.54	0.41
3:4:257:GLY:HA2	36:4:501:GCP:O5'	2.21	0.41
3:4:369:ASN:C	3:4:371:ILE:N	2.73	0.41
4:A:1758:G:O2'	4:A:1759:A:O4'	2.36	0.41
10:G:33:LEU:HB3	10:G:76:LEU:HG	2.02	0.41
1:2:47:ILE:O	1:2:51:HIS:HB3	2.21	0.41
3:4:47:GLU:CA	3:4:79:SER:HB3	2.51	0.41
3:4:171:TYR:CD1	3:4:171:TYR:C	2.95	0.41
3:4:202:GLY:CA	4:A:2676:C:O4'	2.67	0.41
3:4:237:ARG:HE	3:4:240:ARG:NH2	2.19	0.41
3:4:275:ALA:C	3:4:276:LEU:HD12	2.40	0.41
4:A:2902:A:H2'	4:A:2903:A:C8	2.56	0.41
3:4:43:GLN:HA	3:4:43:GLN:HE21	1.85	0.41
3:4:148:LEU:HA	3:4:311:LEU:CD1	2.49	0.41
3:4:199:GLY:CA	3:4:201:ARG:CD	2.98	0.41
3:4:334:GLY:C	3:4:336:ASP:H	2.24	0.41
3:4:337:VAL:HG23	3:4:338:ASN:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:406:ARG:HA	3:4:409:GLU:CD	2.42	0.41
4:A:368:U:O2	4:A:434:G:N2	2.44	0.41
3:4:141:ILE:HG22	3:4:145:ALA:HB3	2.04	0.40
3:4:440:ASP:HB3	3:4:453:ALA:HA	2.03	0.40
4:A:159:A:N3	4:A:2431:C:O2'	2.42	0.40
4:A:2314:U:H4'	28:Y:56:ILE:HD11	2.03	0.40
8:E:101:ARG:HH11	8:E:101:ARG:HD3	1.76	0.40
14:K:92:LEU:HA	14:K:92:LEU:HD23	1.89	0.40
20:Q:3:THR:HG23	20:Q:4:LEU:HG	2.02	0.40
3:4:250:ILE:CG2	3:4:299:ASP:HA	2.51	0.40
3:4:261:LEU:HD13	3:4:261:LEU:HA	1.93	0.40
3:4:371:ILE:CG2	3:4:391:PHE:CD2	3.03	0.40
4:A:2601:A:HO2'	4:A:2602:A:H8	1.68	0.40
4:A:2905:C:OP2	7:D:119:LYS:NZ	2.52	0.40
28:Y:5:CYS:SG	28:Y:8:CYS:N	2.75	0.40
3:4:42:ARG:NH1	3:4:44:LEU:CB	2.79	0.40
3:4:52:VAL:HG12	3:4:106:LEU:HD11	2.03	0.40
3:4:178:GLY:C	3:4:180:GLY:N	2.73	0.40
3:4:215:ILE:HG23	3:4:216:ARG:N	2.35	0.40
3:4:288:GLU:HA	3:4:295:PHE:HD2	1.87	0.40
3:4:290:GLU:CD	3:4:291:ASP:N	2.75	0.40
16:M:137:ILE:HG21	16:M:144:ALA:HB2	2.03	0.40
3:4:462:THR:O	3:4:463:LEU:C	2.60	0.40
26:W:109:GLU:HG2	26:W:130:THR:HB	2.04	0.40
3:4:371:ILE:CG2	3:4:372:ASP:H	2.28	0.40
4:A:978:A:H2'	4:A:979:G:H8	1.86	0.40
4:A:1007:G:N1	4:A:1008:G:N3	2.70	0.40
4:A:2599:G:N2	4:A:2601:A:O2'	2.55	0.40
9:F:43:VAL:HG13	9:F:161:ILE:HG22	2.02	0.40
14:K:7:LYS:HD3	14:K:7:LYS:HA	1.77	0.40
17:N:71:ASP:N	17:N:71:ASP:OD1	2.55	0.40
19:P:50:GLN:HB2	19:P:63:ALA:N	2.36	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	
1	2	57/61 (93%)	56 (98%)	1 (2%)	0	100	100
2	3	21/24 (88%)	20 (95%)	1 (5%)	0	100	100
3	4	424/470 (90%)	343 (81%)	79 (19%)	2 (0%)	25	55
6	C	273/278 (98%)	258 (94%)	15 (6%)	0	100	100
7	D	212/217 (98%)	196 (92%)	16 (8%)	0	100	100
8	E	207/215 (96%)	192 (93%)	15 (7%)	0	100	100
9	F	180/187 (96%)	146 (81%)	34 (19%)	0	100	100
10	G	174/179 (97%)	151 (87%)	23 (13%)	0	100	100
11	H	149/151 (99%)	110 (74%)	39 (26%)	0	100	100
12	I	124/175 (71%)	108 (87%)	16 (13%)	0	100	100
13	J	131/142 (92%)	100 (76%)	31 (24%)	0	100	100
14	K	144/147 (98%)	137 (95%)	7 (5%)	0	100	100
15	L	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
16	M	143/147 (97%)	130 (91%)	13 (9%)	0	100	100
17	N	134/138 (97%)	124 (92%)	10 (8%)	0	100	100
18	O	116/199 (58%)	107 (92%)	9 (8%)	0	100	100
19	P	124/127 (98%)	88 (71%)	36 (29%)	0	100	100
20	Q	111/113 (98%)	95 (86%)	16 (14%)	0	100	100
21	R	122/129 (95%)	118 (97%)	4 (3%)	0	100	100
22	S	98/103 (95%)	92 (94%)	6 (6%)	0	100	100
23	T	112/153 (73%)	110 (98%)	2 (2%)	0	100	100
24	U	95/100 (95%)	90 (95%)	5 (5%)	0	100	100
25	V	93/105 (89%)	82 (88%)	11 (12%)	0	100	100
26	W	190/215 (88%)	170 (90%)	20 (10%)	0	100	100
27	X	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
28	Y	61/64 (95%)	55 (90%)	6 (10%)	0	100	100
29	Z	62/77 (80%)	62 (100%)	0	0	100	100
30	b	52/57 (91%)	52 (100%)	0	0	100	100
31	c	47/55 (86%)	45 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	d	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
33	e	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
34	f	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
35	g	46/75 (61%)	41 (89%)	5 (11%)	0	100	100
All	All	4039/4461 (90%)	3594 (89%)	443 (11%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	4	294	PRO
3	4	431	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	52/54 (96%)	52 (100%)	0	100	100
2	3	18/19 (95%)	18 (100%)	0	100	100
3	4	337/372 (91%)	310 (92%)	27 (8%)	10	31
6	C	215/218 (99%)	214 (100%)	1 (0%)	86	92
7	D	160/163 (98%)	160 (100%)	0	100	100
8	E	169/173 (98%)	169 (100%)	0	100	100
9	F	151/156 (97%)	149 (99%)	2 (1%)	65	80
10	G	148/150 (99%)	145 (98%)	3 (2%)	50	71
11	H	90/116 (78%)	90 (100%)	0	100	100
12	I	89/120 (74%)	89 (100%)	0	100	100
13	J	102/108 (94%)	100 (98%)	2 (2%)	50	71
14	K	119/120 (99%)	119 (100%)	0	100	100
15	L	100/100 (100%)	99 (99%)	1 (1%)	73	85
16	M	112/114 (98%)	111 (99%)	1 (1%)	75	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	N	114/116 (98%)	112 (98%)	2 (2%)	54	74
18	O	97/158 (61%)	97 (100%)	0	100	100
19	P	93/94 (99%)	88 (95%)	5 (5%)	18	44
20	Q	100/100 (100%)	100 (100%)	0	100	100
21	R	97/99 (98%)	97 (100%)	0	100	100
22	S	81/83 (98%)	81 (100%)	0	100	100
23	T	90/117 (77%)	89 (99%)	1 (1%)	70	83
24	U	83/85 (98%)	83 (100%)	0	100	100
25	V	81/86 (94%)	80 (99%)	1 (1%)	67	81
26	W	155/168 (92%)	155 (100%)	0	100	100
27	X	58/63 (92%)	57 (98%)	1 (2%)	56	75
28	Y	50/51 (98%)	49 (98%)	1 (2%)	50	71
29	Z	58/66 (88%)	57 (98%)	1 (2%)	56	75
30	b	43/46 (94%)	43 (100%)	0	100	100
31	c	47/52 (90%)	47 (100%)	0	100	100
32	d	35/36 (97%)	35 (100%)	0	100	100
33	e	53/54 (98%)	53 (100%)	0	100	100
34	f	35/35 (100%)	35 (100%)	0	100	100
35	g	43/63 (68%)	43 (100%)	0	100	100
All	All	3275/3555 (92%)	3226 (98%)	49 (2%)	60	78

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	4	46	LEU
3	4	56	THR
3	4	57	GLU
3	4	64	GLU
3	4	85	LEU
3	4	98	ILE
3	4	106	LEU
3	4	140	VAL
3	4	147	ILE
3	4	148	LEU
3	4	172	MET

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Mol	Chain	Res	Type
3	4	186	GLN
3	4	201	ARG
3	4	218	ARG
3	4	226	ILE
3	4	274	ASN
3	4	283	THR
3	4	295	PHE
3	4	311	LEU
3	4	384	ARG
3	4	391	PHE
3	4	430	VAL
3	4	438	HIS
3	4	439	VAL
3	4	446	ASP
3	4	450	ARG
3	4	464	ARG
6	C	134	ARG
9	F	52	ARG
9	F	74	VAL
10	G	36	ASP
10	G	45	ARG
10	G	66	HIS
13	J	108	ARG
13	J	135	ARG
15	L	73	ASP
16	M	49	MET
17	N	60	ARG
17	N	120	ARG
19	P	45	ARG
19	P	47	ILE
19	P	50	GLN
19	P	51	LEU
19	P	108	THR
23	T	99	ARG
25	V	44	HIS
27	X	14	ARG
28	Y	5	CYS
29	Z	58	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
3	4	43	GLN
3	4	87	GLN
3	4	128	GLN
3	4	154	HIS
3	4	434	HIS
3	4	444	HIS
6	C	91	ASN
6	C	261	ASN
7	D	34	ASN
8	E	100	GLN
9	F	58	ASN
9	F	62	ASN
10	G	103	ASN
11	H	102	ASN
11	H	118	GLN
12	I	54	ASN
13	J	14	GLN
13	J	21	ASN
13	J	36	ASN
13	J	45	ASN
14	K	132	HIS
14	K	144	GLN
15	L	91	ASN
16	M	76	GLN
19	P	16	ASN
21	R	39	GLN
22	S	76	HIS
22	S	90	HIS
23	T	67	ASN
23	T	109	HIS
24	U	34	HIS
24	U	41	GLN
26	W	14	ASN
26	W	46	HIS
26	W	76	GLN
27	X	50	ASN
35	g	40	GLN
35	g	42	HIS

5.3.3 RNA ⓘ

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	A	3118/3120 (99%)	760 (24%)	22 (0%)
5	B	117/118 (99%)	37 (31%)	2 (1%)
All	All	3235/3238 (99%)	797 (24%)	24 (0%)

All (797) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	A	7	U
4	A	9	U
4	A	11	A
4	A	12	G
4	A	20	G
4	A	31	U
4	A	32	G
4	A	33	G
4	A	42	G
4	A	46	A
4	A	48	G
4	A	55	G
4	A	58	G
4	A	60	A
4	A	68	A
4	A	71	A
4	A	72	G
4	A	80	G
4	A	81	A
4	A	88	A
4	A	91	C
4	A	94	G
4	A	95	C
4	A	98	U
4	A	99	G
4	A	107	G
4	A	115	A
4	A	116	A
4	A	117	U
4	A	122	A
4	A	125	C
4	A	137	G
4	A	162	A
4	A	164	A

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Mol	Chain	Res	Type
4	A	180	A
4	A	195	A
4	A	198	A
4	A	200	C
4	A	203	A
4	A	212	A
4	A	214	G
4	A	215	A
4	A	220	A
4	A	221	A
4	A	227	A
4	A	229	U
4	A	230	G
4	A	241	A
4	A	248	G
4	A	266	U
4	A	267	G
4	A	273	A
4	A	274	C
4	A	276	G
4	A	280	G
4	A	281	C
4	A	286	G
4	A	288	U
4	A	289	A
4	A	290	C
4	A	292	G
4	A	296	A
4	A	299	G
4	A	300	G
4	A	302	U
4	A	303	G
4	A	305	G
4	A	306	U
4	A	307	G
4	A	309	G
4	A	314	G
4	A	315	U
4	A	316	U
4	A	317	G
4	A	318	U
4	A	319	G

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Mol	Chain	Res	Type
4	A	325	U
4	A	326	A
4	A	327	U
4	A	329	U
4	A	330	U
4	A	331	U
4	A	334	G
4	A	337	U
4	A	338	C
4	A	340	A
4	A	341	C
4	A	342	C
4	A	344	G
4	A	351	G
4	A	357	U
4	A	358	G
4	A	361	A
4	A	363	A
4	A	364	A
4	A	366	G
4	A	370	U
4	A	371	G
4	A	382	A
4	A	384	G
4	A	391	G
4	A	393	U
4	A	399	G
4	A	405	G
4	A	412	A
4	A	413	G
4	A	415	G
4	A	416	C
4	A	427	A
4	A	437	G
4	A	438	U
4	A	441	G
4	A	445	U
4	A	446	G
4	A	451	U
4	A	453	U
4	A	460	G
4	A	474	G

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Mol	Chain	Res	Type
4	A	489	A
4	A	492	C
4	A	493	U
4	A	494	G
4	A	511	A
4	A	512	G
4	A	543	U
4	A	544	U
4	A	555	G
4	A	563	U
4	A	566	A
4	A	567	A
4	A	569	G
4	A	570	U
4	A	571	A
4	A	572	C
4	A	573	C
4	A	578	G
4	A	581	G
4	A	591	G
4	A	592	A
4	A	593	G
4	A	594	U
4	A	595	A
4	A	596	C
4	A	605	G
4	A	612	U
4	A	617	U
4	A	618	C
4	A	619	C
4	A	620	G
4	A	633	A
4	A	635	G
4	A	636	U
4	A	637	G
4	A	639	C
4	A	640	G
4	A	642	G
4	A	644	G
4	A	655	G
4	A	665	G
4	A	667	A

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Mol	Chain	Res	Type
4	A	678	A
4	A	679	G
4	A	684	G
4	A	696	A
4	A	706	G
4	A	707	G
4	A	708	G
4	A	709	U
4	A	721	A
4	A	725	A
4	A	728	G
4	A	731	A
4	A	736	G
4	A	737	A
4	A	739	U
4	A	740	A
4	A	742	G
4	A	747	A
4	A	748	U
4	A	757	G
4	A	758	A
4	A	759	G
4	A	760	U
4	A	763	G
4	A	765	G
4	A	766	G
4	A	768	G
4	A	769	U
4	A	801	U
4	A	826	G
4	A	830	A
4	A	831	A
4	A	842	A
4	A	843	G
4	A	845	C
4	A	862	U
4	A	868	C
4	A	872	G
4	A	877	U
4	A	879	A
4	A	880	G
4	A	890	G

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Mol	Chain	Res	Type
4	A	891	G
4	A	897	A
4	A	899	G
4	A	904	A
4	A	908	A
4	A	919	A
4	A	920	G
4	A	927	C
4	A	942	U
4	A	944	A
4	A	974	G
4	A	975	U
4	A	981	U
4	A	982	A
4	A	990	G
4	A	994	A
4	A	995	U
4	A	996	G
4	A	1001	C
4	A	1002	C
4	A	1004	C
4	A	1005	A
4	A	1006	G
4	A	1008	G
4	A	1010	U
4	A	1011	A
4	A	1012	C
4	A	1014	G
4	A	1016	C
4	A	1025	A
4	A	1027	C
4	A	1046	C
4	A	1047	A
4	A	1048	A
4	A	1049	G
4	A	1063	G
4	A	1074	A
4	A	1076	A
4	A	1078	G
4	A	1085	G
4	A	1091	A
4	A	1092	G

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Mol	Chain	Res	Type
4	A	1097	A
4	A	1101	A
4	A	1114	G
4	A	1127	A
4	A	1130	C
4	A	1131	G
4	A	1143	G
4	A	1144	A
4	A	1148	G
4	A	1151	U
4	A	1156	A
4	A	1162	G
4	A	1163	A
4	A	1164	A
4	A	1165	G
4	A	1167	C
4	A	1171	C
4	A	1172	A
4	A	1173	G
4	A	1174	G
4	A	1175	A
4	A	1176	G
4	A	1178	U
4	A	1179	U
4	A	1180	G
4	A	1181	G
4	A	1182	C
4	A	1184	U
4	A	1185	A
4	A	1186	G
4	A	1187	A
4	A	1188	A
4	A	1190	C
4	A	1191	A
4	A	1195	A
4	A	1196	C
4	A	1197	C
4	A	1198	C
4	A	1199	U
4	A	1200	U
4	A	1201	G
4	A	1202	A

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Mol	Chain	Res	Type
4	A	1203	A
4	A	1204	A
4	A	1205	G
4	A	1206	A
4	A	1207	G
4	A	1212	U
4	A	1213	A
4	A	1214	A
4	A	1216	A
4	A	1217	G
4	A	1219	U
4	A	1222	C
4	A	1225	G
4	A	1226	U
4	A	1227	C
4	A	1228	A
4	A	1229	A
4	A	1230	G
4	A	1231	U
4	A	1236	G
4	A	1237	U
4	A	1238	G
4	A	1239	C
4	A	1240	G
4	A	1246	A
4	A	1248	U
4	A	1251	A
4	A	1253	C
4	A	1254	G
4	A	1260	C
4	A	1261	A
4	A	1270	G
4	A	1275	A
4	A	1292	U
4	A	1293	G
4	A	1332	G
4	A	1343	G
4	A	1344	A
4	A	1353	G
4	A	1362	A
4	A	1365	G
4	A	1371	G

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Mol	Chain	Res	Type
4	A	1377	A
4	A	1380	A
4	A	1386	G
4	A	1387	A
4	A	1389	U
4	A	1399	A
4	A	1401	A
4	A	1402	A
4	A	1404	C
4	A	1415	A
4	A	1416	A
4	A	1436	C
4	A	1444	U
4	A	1456	G
4	A	1465	C
4	A	1467	U
4	A	1480	A
4	A	1493	A
4	A	1494	U
4	A	1499	A
4	A	1508	A
4	A	1510	A
4	A	1518	A
4	A	1522	G
4	A	1530	G
4	A	1531	C
4	A	1532	G
4	A	1533	U
4	A	1535	C
4	A	1536	A
4	A	1538	G
4	A	1542	A
4	A	1546	A
4	A	1548	C
4	A	1549	G
4	A	1550	G
4	A	1551	U
4	A	1553	C
4	A	1556	A
4	A	1564	A
4	A	1566	A
4	A	1567	C

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Mol	Chain	Res	Type
4	A	1573	U
4	A	1574	G
4	A	1575	A
4	A	1577	C
4	A	1578	G
4	A	1580	A
4	A	1582	C
4	A	1583	U
4	A	1584	U
4	A	1585	U
4	A	1586	C
4	A	1587	G
4	A	1588	G
4	A	1589	G
4	A	1592	G
4	A	1593	U
4	A	1597	G
4	A	1598	U
4	A	1599	U
4	A	1600	G
4	A	1601	G
4	A	1603	G
4	A	1608	U
4	A	1609	G
4	A	1610	C
4	A	1616	A
4	A	1617	C
4	A	1618	C
4	A	1619	U
4	A	1621	C
4	A	1622	G
4	A	1623	U
4	A	1624	U
4	A	1625	G
4	A	1628	A
4	A	1629	G
4	A	1630	U
4	A	1632	G
4	A	1636	A
4	A	1638	C
4	A	1640	A
4	A	1648	A

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Mol	Chain	Res	Type
4	A	1649	C
4	A	1670	G
4	A	1671	U
4	A	1673	A
4	A	1674	G
4	A	1676	G
4	A	1678	U
4	A	1679	A
4	A	1681	U
4	A	1688	G
4	A	1703	G
4	A	1708	A
4	A	1709	U
4	A	1710	A
4	A	1713	U
4	A	1716	A
4	A	1717	U
4	A	1718	C
4	A	1723	U
4	A	1728	U
4	A	1730	U
4	A	1731	A
4	A	1737	A
4	A	1744	A
4	A	1746	G
4	A	1754	G
4	A	1756	G
4	A	1757	U
4	A	1759	A
4	A	1767	U
4	A	1768	C
4	A	1769	G
4	A	1777	U
4	A	1778	A
4	A	1786	G
4	A	1787	A
4	A	1789	A
4	A	1798	U
4	A	1803	A
4	A	1813	C
4	A	1825	C
4	A	1826	A

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Mol	Chain	Res	Type
4	A	1835	C
4	A	1844	A
4	A	1847	U
4	A	1848	A
4	A	1851	G
4	A	1852	A
4	A	1864	U
4	A	1866	C
4	A	1871	G
4	A	1872	A
4	A	1892	G
4	A	1893	C
4	A	1904	C
4	A	1911	U
4	A	1912	C
4	A	1916	A
4	A	1931	A
4	A	1940	A
4	A	1941	A
4	A	1942	G
4	A	1943	C
4	A	1945	U
4	A	1946	U
4	A	1947	U
4	A	1948	A
4	A	1949	C
4	A	1955	A
4	A	1961	G
4	A	1972	A
4	A	1973	C
4	A	1975	A
4	A	1981	U
4	A	1990	A
4	A	1999	U
4	A	2017	C
4	A	2018	G
4	A	2026	A
4	A	2033	U
4	A	2046	A
4	A	2075	G
4	A	2083	A
4	A	2085	C

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Mol	Chain	Res	Type
4	A	2086	U
4	A	2089	C
4	A	2092	U
4	A	2093	G
4	A	2094	G
4	A	2095	G
4	A	2107	G
4	A	2113	A
4	A	2128	G
4	A	2130	G
4	A	2131	G
4	A	2132	U
4	A	2133	G
4	A	2134	G
4	A	2135	U
4	A	2136	A
4	A	2137	A
4	A	2138	C
4	A	2139	U
4	A	2140	A
4	A	2141	U
4	A	2142	A
4	A	2145	C
4	A	2146	A
4	A	2147	U
4	A	2148	C
4	A	2151	A
4	A	2152	A
4	A	2153	G
4	A	2154	G
4	A	2160	A
4	A	2161	A
4	A	2162	A
4	A	2163	U
4	A	2179	U
4	A	2187	U
4	A	2190	A
4	A	2191	C
4	A	2194	A
4	A	2195	U
4	A	2196	G
4	A	2215	U

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Mol	Chain	Res	Type
4	A	2216	G
4	A	2217	U
4	A	2221	A
4	A	2227	A
4	A	2246	U
4	A	2247	A
4	A	2251	G
4	A	2254	A
4	A	2255	A
4	A	2256	G
4	A	2257	A
4	A	2263	G
4	A	2267	C
4	A	2276	G
4	A	2279	C
4	A	2280	G
4	A	2284	A
4	A	2285	G
4	A	2286	A
4	A	2310	G
4	A	2316	G
4	A	2320	C
4	A	2321	U
4	A	2323	G
4	A	2326	A
4	A	2327	C
4	A	2329	G
4	A	2330	U
4	A	2332	U
4	A	2333	G
4	A	2334	U
4	A	2335	G
4	A	2336	U
4	A	2339	G
4	A	2340	A
4	A	2341	U
4	A	2342	A
4	A	2343	G
4	A	2345	U
4	A	2346	G
4	A	2348	G
4	A	2350	G

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Mol	Chain	Res	Type
4	A	2351	A
4	A	2353	U
4	A	2354	G
4	A	2355	U
4	A	2356	G
4	A	2357	A
4	A	2358	A
4	A	2362	C
4	A	2363	A
4	A	2365	A
4	A	2366	C
4	A	2367	G
4	A	2368	C
4	A	2369	C
4	A	2371	G
4	A	2374	U
4	A	2376	G
4	A	2379	G
4	A	2380	G
4	A	2381	A
4	A	2382	G
4	A	2384	C
4	A	2385	G
4	A	2386	U
4	A	2387	U
4	A	2388	G
4	A	2389	U
4	A	2390	U
4	A	2391	G
4	A	2392	A
4	A	2393	A
4	A	2394	A
4	A	2395	U
4	A	2396	A
4	A	2398	C
4	A	2399	A
4	A	2400	C
4	A	2401	U
4	A	2402	C
4	A	2403	U
4	A	2405	A
4	A	2407	C

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Mol	Chain	Res	Type
4	A	2410	A
4	A	2413	G
4	A	2421	A
4	A	2422	A
4	A	2434	A
4	A	2446	G
4	A	2449	A
4	A	2462	G
4	A	2463	G
4	A	2467	U
4	A	2470	A
4	A	2474	G
4	A	2475	G
4	A	2476	G
4	A	2483	G
4	A	2490	A
4	A	2492	A
4	A	2503	G
4	A	2506	G
4	A	2507	C
4	A	2511	A
4	A	2516	U
4	A	2528	G
4	A	2529	A
4	A	2531	G
4	A	2532	G
4	A	2533	C
4	A	2534	A
4	A	2535	A
4	A	2536	U
4	A	2538	A
4	A	2544	U
4	A	2545	G
4	A	2549	G
4	A	2559	A
4	A	2567	U
4	A	2569	G
4	A	2571	C
4	A	2572	U
4	A	2574	C
4	A	2582	A
4	A	2585	U

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Mol	Chain	Res	Type
4	A	2600	A
4	A	2601	A
4	A	2602	A
4	A	2607	G
4	A	2609	A
4	A	2620	G
4	A	2630	A
4	A	2631	G
4	A	2646	C
4	A	2647	U
4	A	2649	A
4	A	2653	G
4	A	2654	A
4	A	2655	U
4	A	2656	A
4	A	2657	A
4	A	2659	A
4	A	2665	C
4	A	2672	A
4	A	2676	C
4	A	2683	A
4	A	2694	G
4	A	2698	C
4	A	2700	A
4	A	2702	A
4	A	2715	U
4	A	2718	G
4	A	2726	G
4	A	2728	U
4	A	2729	G
4	A	2742	A
4	A	2744	C
4	A	2749	G
4	A	2753	G
4	A	2759	G
4	A	2780	C
4	A	2786	U
4	A	2790	A
4	A	2791	G
4	A	2796	A
4	A	2797	C
4	A	2822	A

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Mol	Chain	Res	Type
4	A	2823	G
4	A	2826	A
4	A	2827	G
4	A	2832	G
4	A	2833	U
4	A	2834	C
4	A	2837	U
4	A	2839	U
4	A	2853	C
4	A	2854	A
4	A	2865	G
4	A	2870	C
4	A	2884	A
4	A	2893	G
4	A	2913	U
4	A	2915	C
4	A	2936	C
4	A	2938	G
4	A	2950	C
4	A	2956	G
4	A	2957	A
4	A	2963	U
4	A	2969	C
4	A	2972	A
4	A	2976	C
4	A	2985	G
4	A	2990	A
4	A	3002	A
4	A	3005	A
4	A	3009	U
4	A	3015	C
4	A	3021	A
4	A	3022	G
4	A	3023	G
4	A	3029	U
4	A	3039	C
4	A	3041	C
4	A	3042	A
4	A	3044	A
4	A	3050	G
4	A	3056	A
4	A	3080	A

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Mol	Chain	Res	Type
4	A	3082	U
4	A	3088	C
4	A	3093	A
4	A	3101	C
4	A	3105	C
4	A	3106	C
4	A	3107	G
4	A	3112	A
4	A	3114	A
4	A	3115	A
4	A	3119	A
4	A	3120	C
5	B	3	U
5	B	4	A
5	B	5	C
5	B	8	C
5	B	9	G
5	B	10	G
5	B	11	U
5	B	13	C
5	B	14	A
5	B	17	G
5	B	23	G
5	B	25	G
5	B	31	C
5	B	33	C
5	B	36	U
5	B	41	U
5	B	42	C
5	B	43	C
5	B	53	A
5	B	56	C
5	B	57	U
5	B	59	A
5	B	66	C
5	B	67	A
5	B	74	A
5	B	86	A
5	B	89	C
5	B	97	A
5	B	100	G
5	B	103	G

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Mol	Chain	Res	Type
5	B	106	C
5	B	107	A
5	B	109	C
5	B	113	G
5	B	114	A
5	B	117	A
5	B	118	C

All (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	A	97	U
4	A	272	A
4	A	336	C
4	A	357	U
4	A	643	G
4	A	842	A
4	A	974	G
4	A	981	U
4	A	1199	U
4	A	1206	A
4	A	1230	G
4	A	1292	U
4	A	1947	U
4	A	2094	G
4	A	2135	U
4	A	2141	U
4	A	2320	C
4	A	2328	G
4	A	2345	U
4	A	2397	C
4	A	2656	A
4	A	2779	U
5	B	10	G
5	B	113	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
36	GCP	4	501	-	27,34,34	1.36	3 (11%)	35,54,54	1.93	7 (20%)

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
36	GCP	4	501	-	-	5/15/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	4	501	GCP	C5-C6	3.99	1.48	1.41
36	4	501	GCP	PG-O2G	2.85	1.61	1.55
36	4	501	GCP	PG-O3G	2.61	1.60	1.55

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	4	501	GCP	C2-N3-C4	4.84	120.70	115.48
36	4	501	GCP	PB-O3A-PA	-4.58	117.42	132.37
36	4	501	GCP	C2-N1-C6	4.23	121.85	115.96
36	4	501	GCP	C5-C6-N1	-3.91	118.19	123.42
36	4	501	GCP	N3-C2-N1	-3.17	123.18	127.21
36	4	501	GCP	C4-C5-N7	-2.86	106.32	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	4	501	GCP	C4-C5-C6	-2.84	116.88	121.23

There are no chirality outliers.

All (5) torsion outliers are listed below:

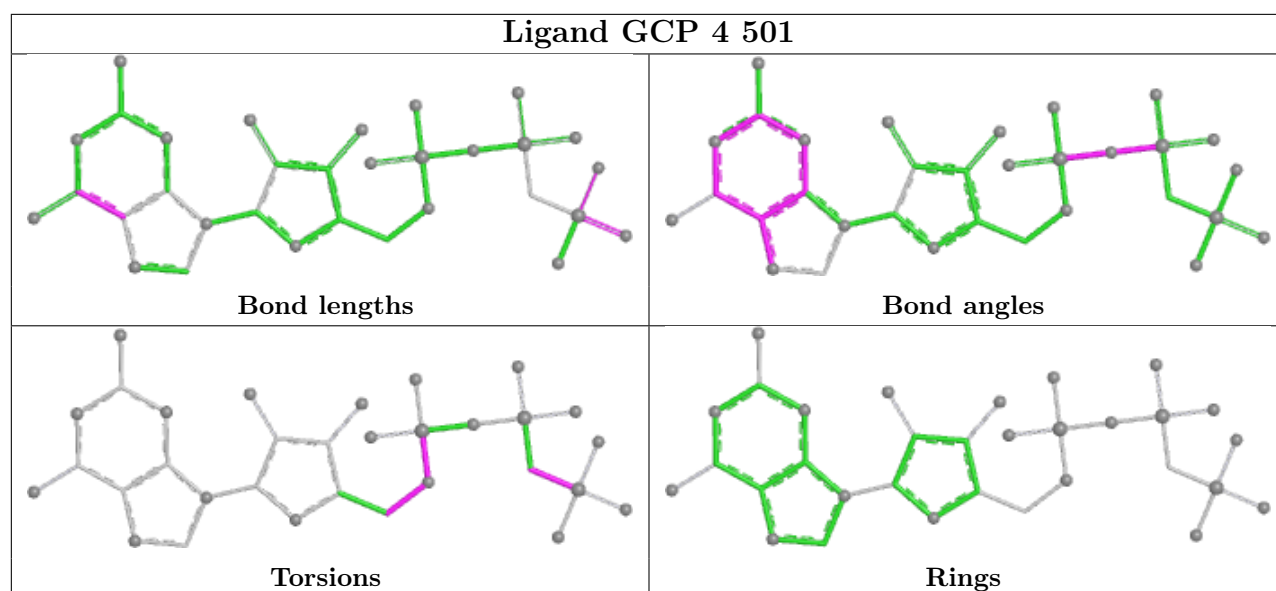
Mol	Chain	Res	Type	Atoms
36	4	501	GCP	PB-C3B-PG-O1G
36	4	501	GCP	PB-C3B-PG-O2G
36	4	501	GCP	PB-C3B-PG-O3G
36	4	501	GCP	C5'-O5'-PA-O1A
36	4	501	GCP	C4'-C5'-O5'-PA

There are no ring outliers.

1 monomer is involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	4	501	GCP	15	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

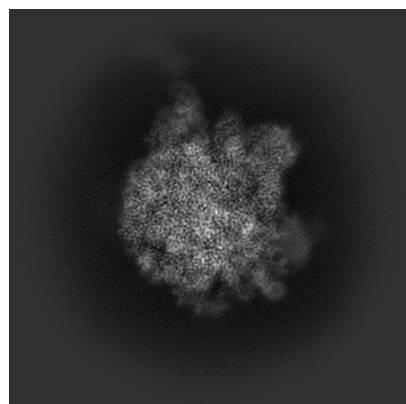
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43294. These allow visual inspection of the internal detail of the map and identification of artifacts.

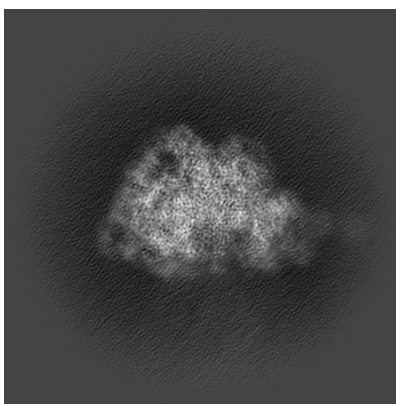
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

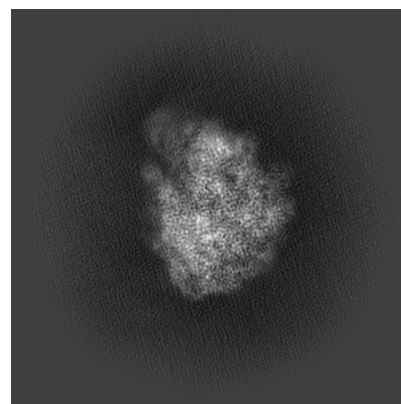
6.1.1 Primary map



X

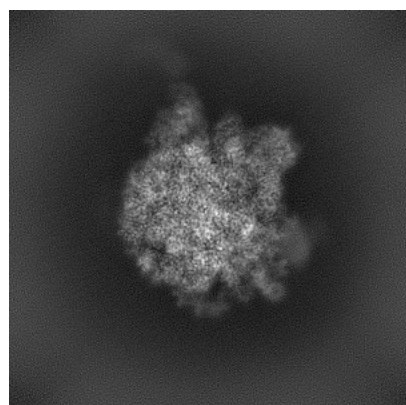


Y

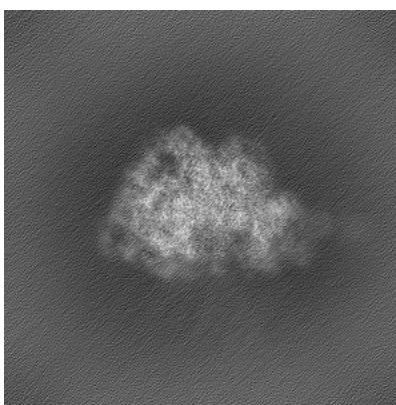


Z

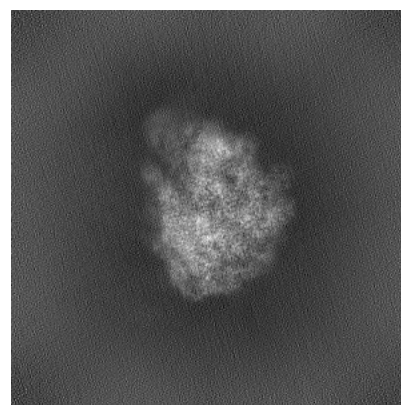
6.1.2 Raw map



X



Y

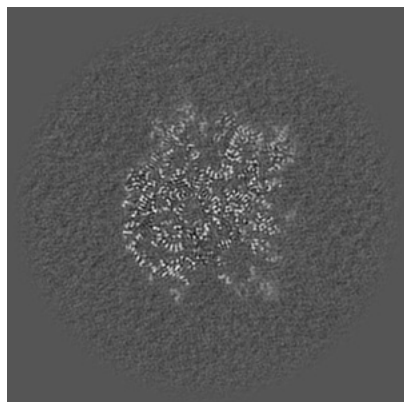


Z

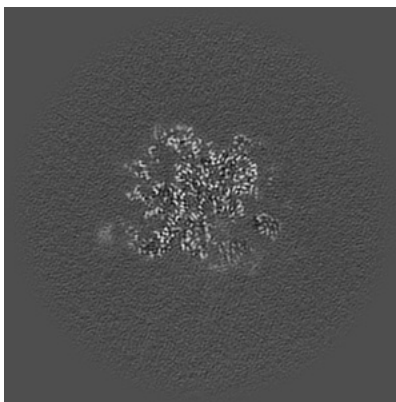
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

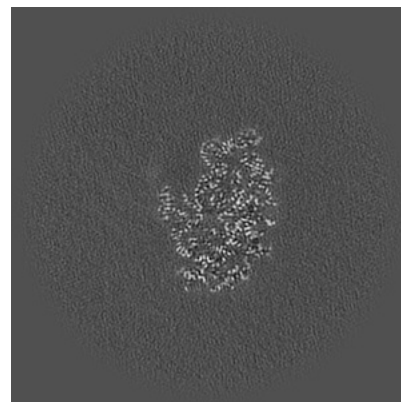
6.2.1 Primary map



X Index: 200

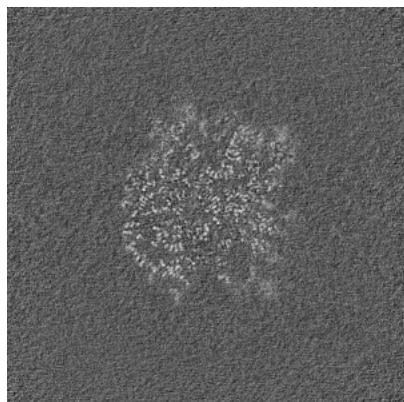


Y Index: 200

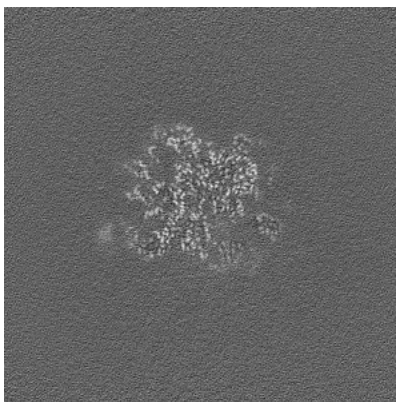


Z Index: 200

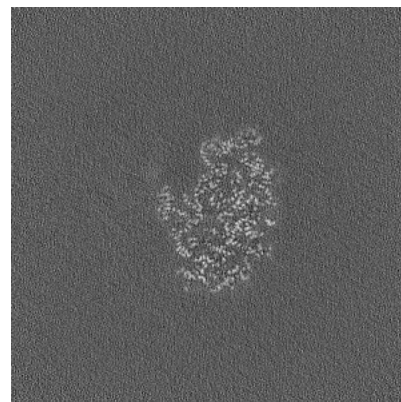
6.2.2 Raw map



X Index: 200



Y Index: 200

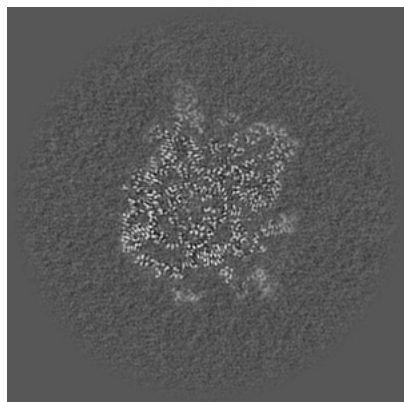


Z Index: 200

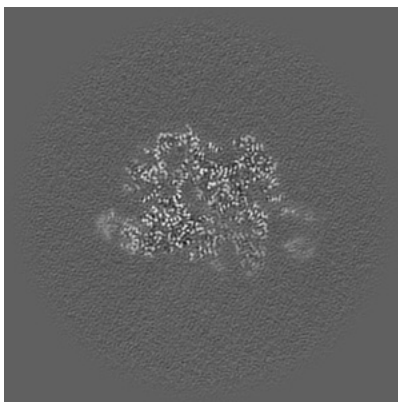
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

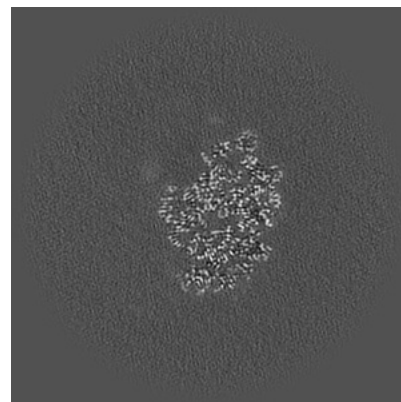
6.3.1 Primary map



X Index: 194

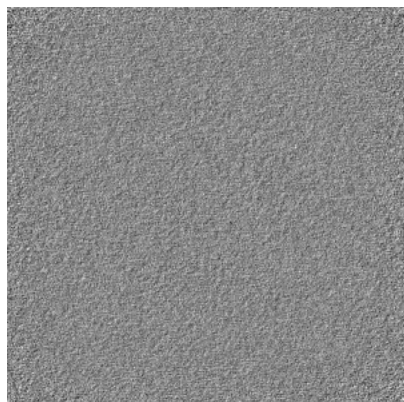


Y Index: 190

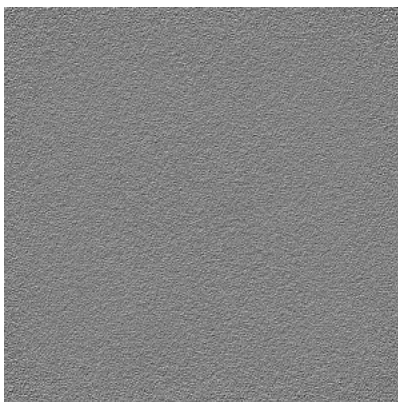


Z Index: 196

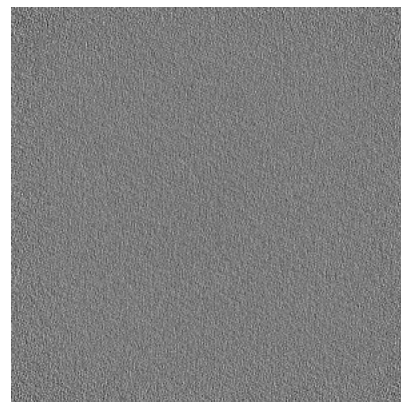
6.3.2 Raw map



X Index: 0



Y Index: 0

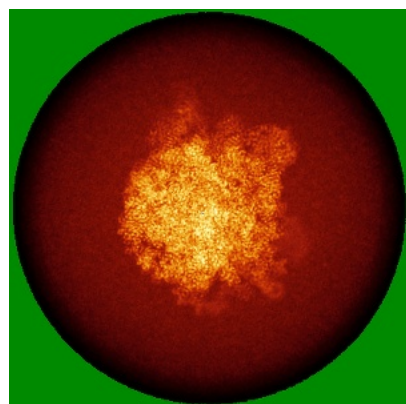


Z Index: 0

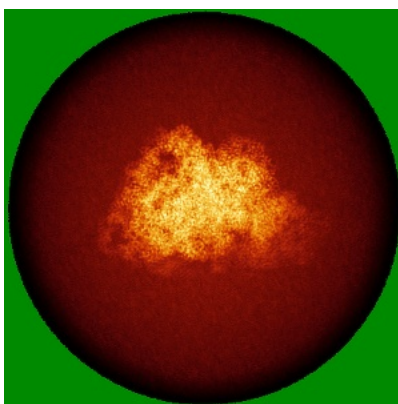
The images above show the largest variance slices of the map in three orthogonal directions.

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

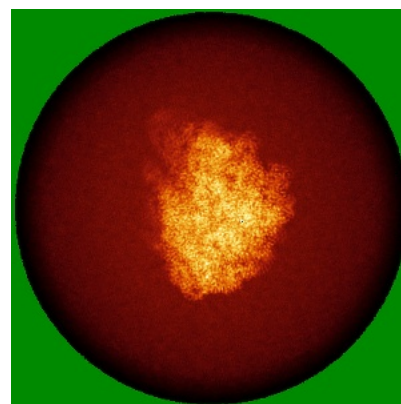
6.4.1 Primary map



X

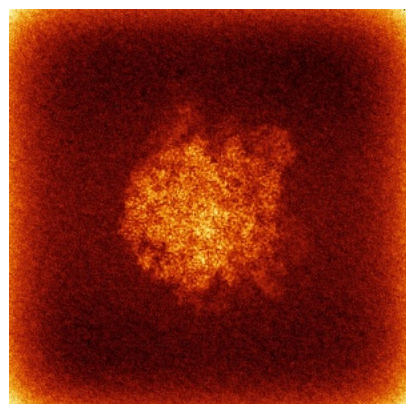


Y

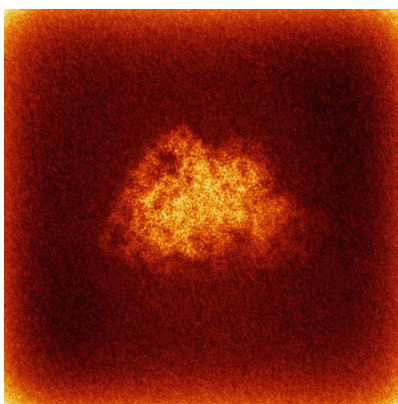


Z

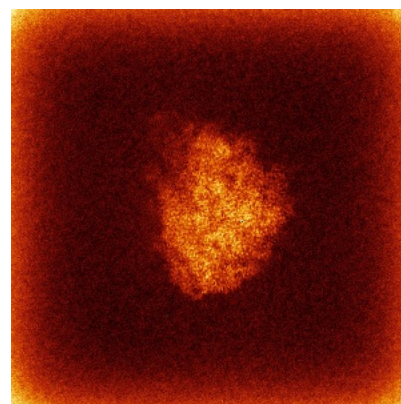
6.4.2 Raw map



X



Y

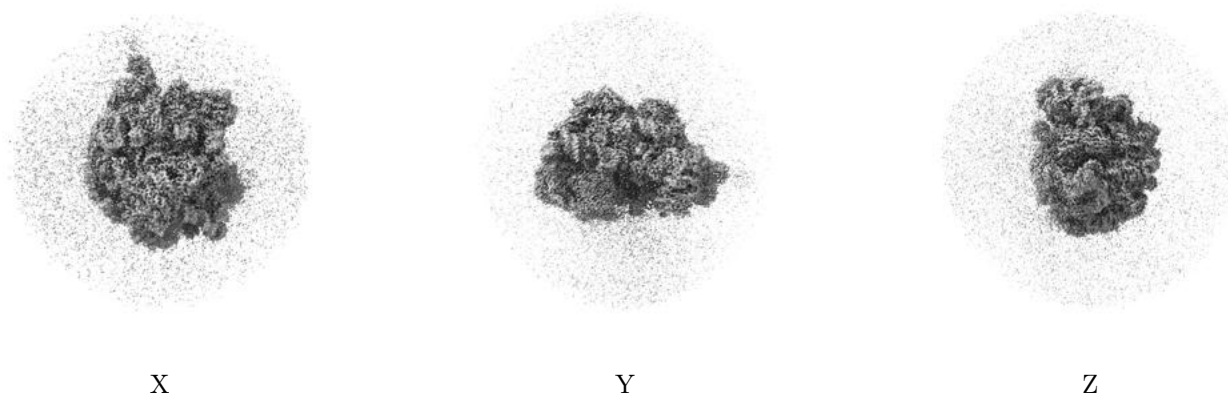


Z

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

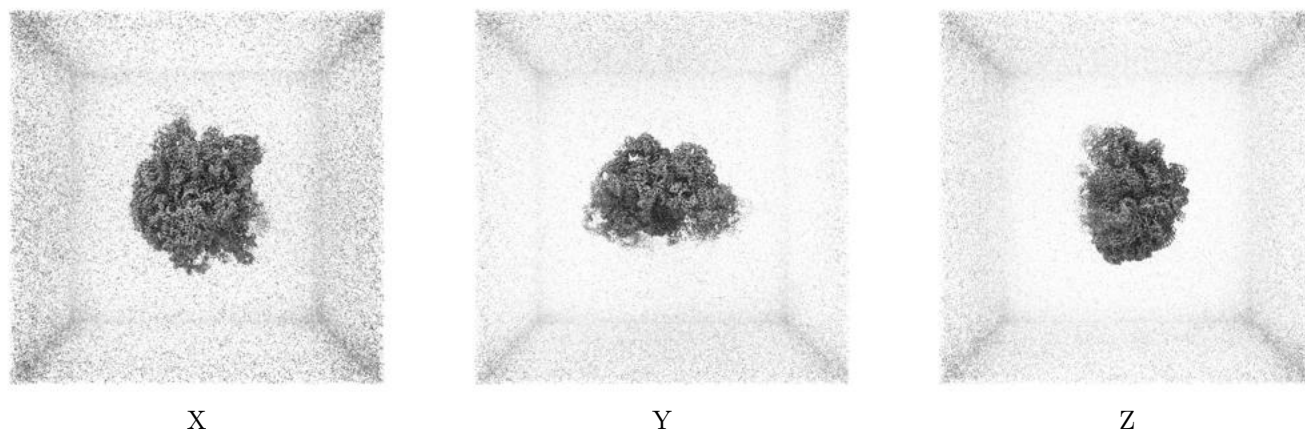
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.19. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

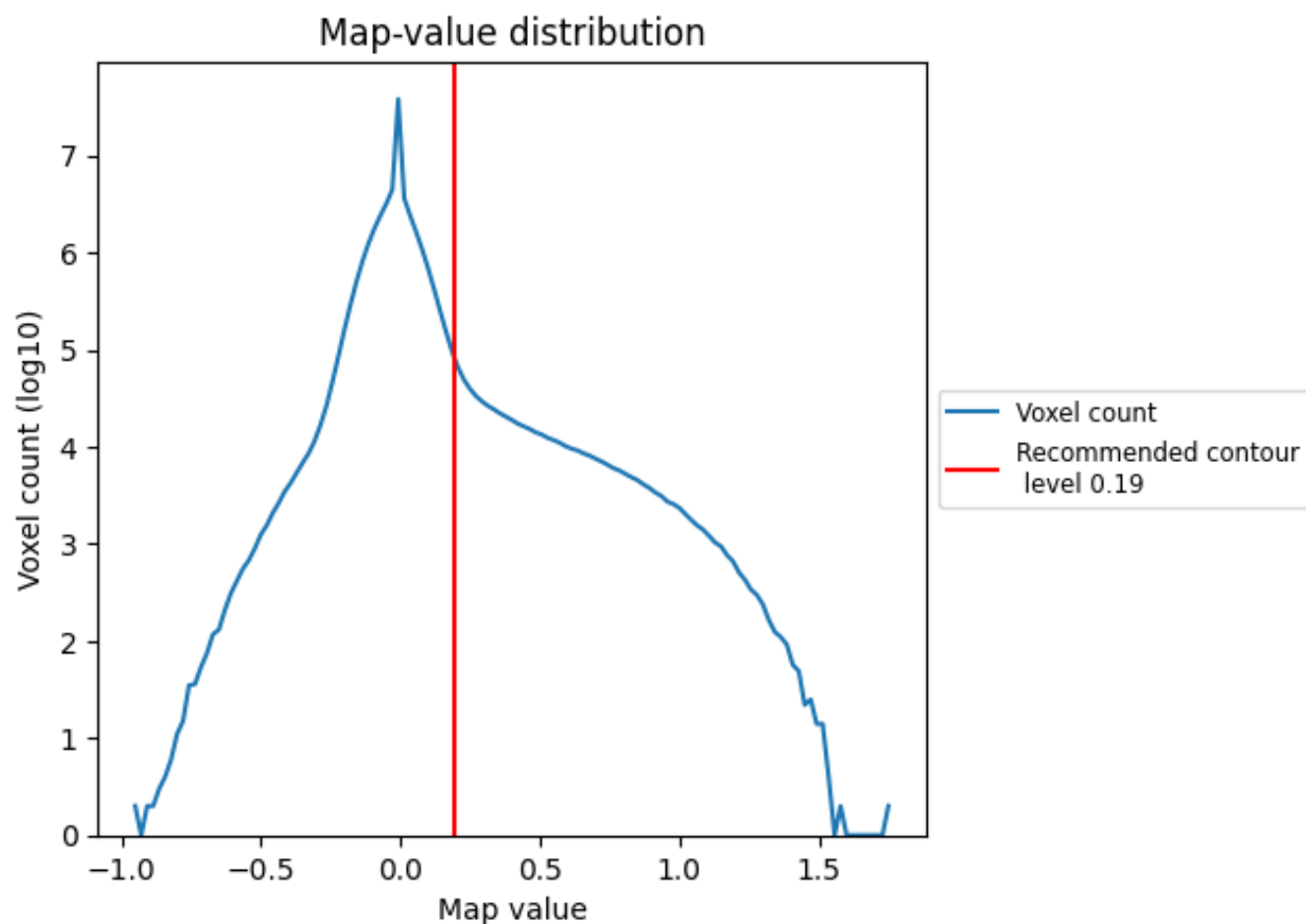
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

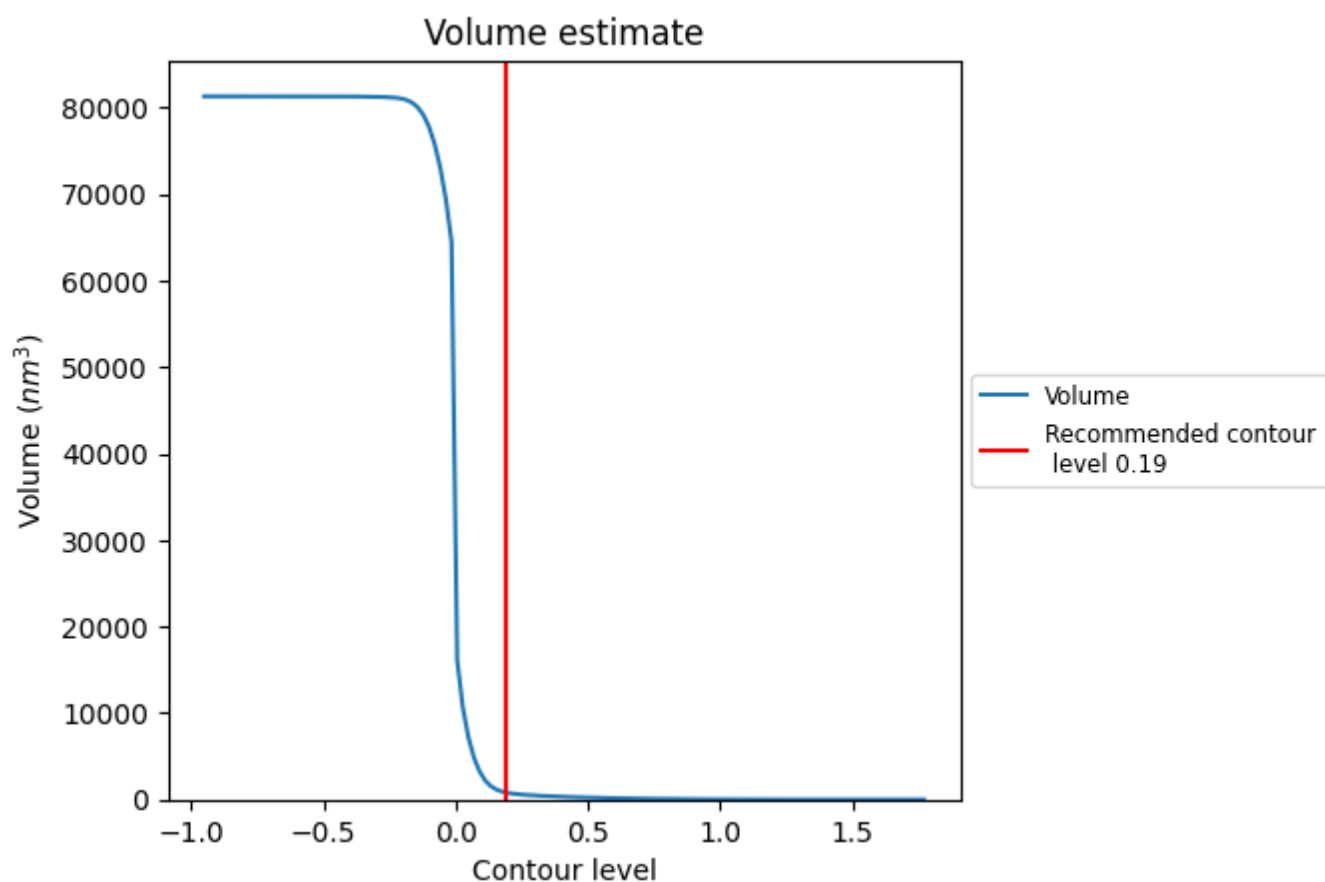
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

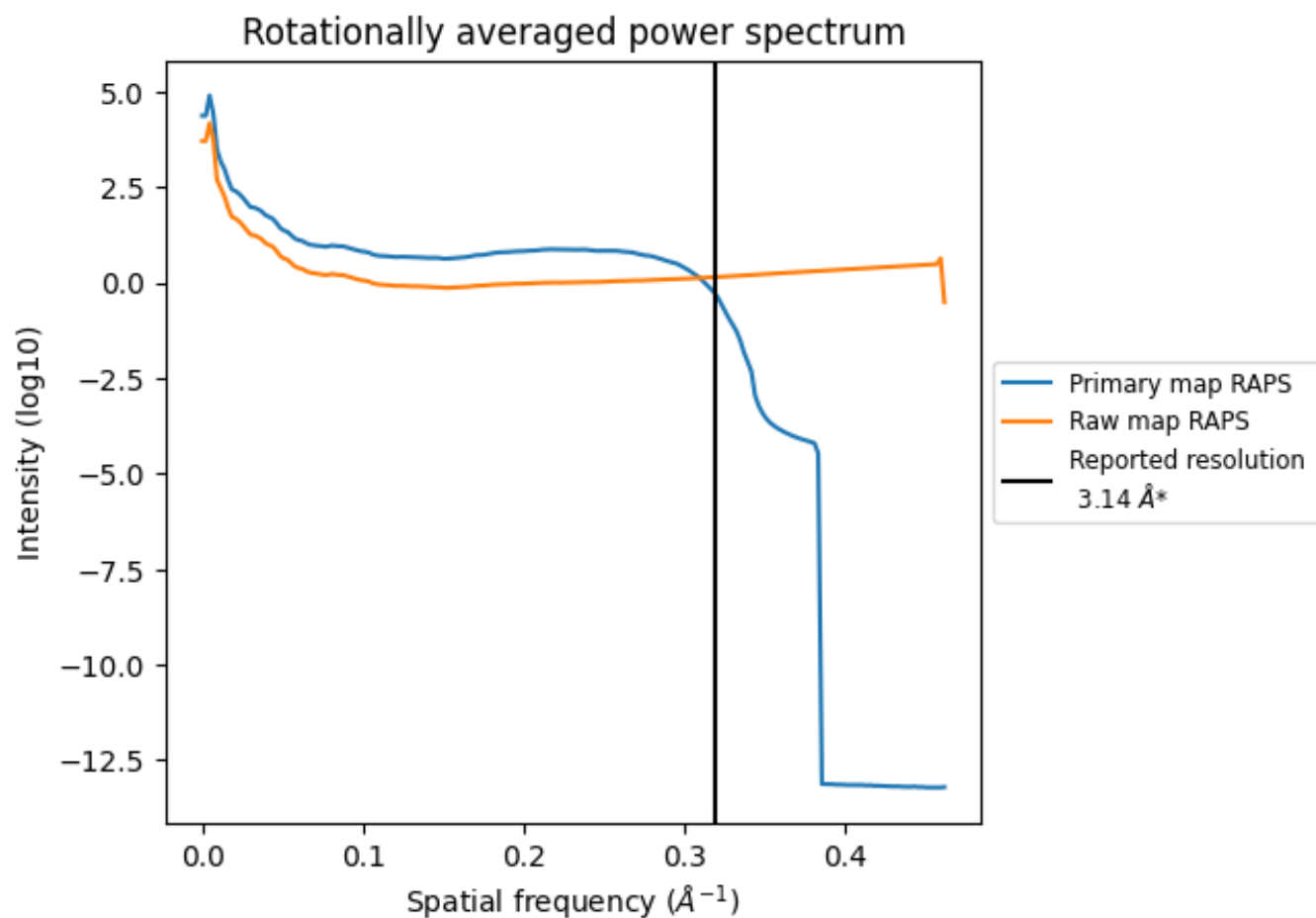
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 817 nm³; this corresponds to an approximate mass of 738 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 ⓘ

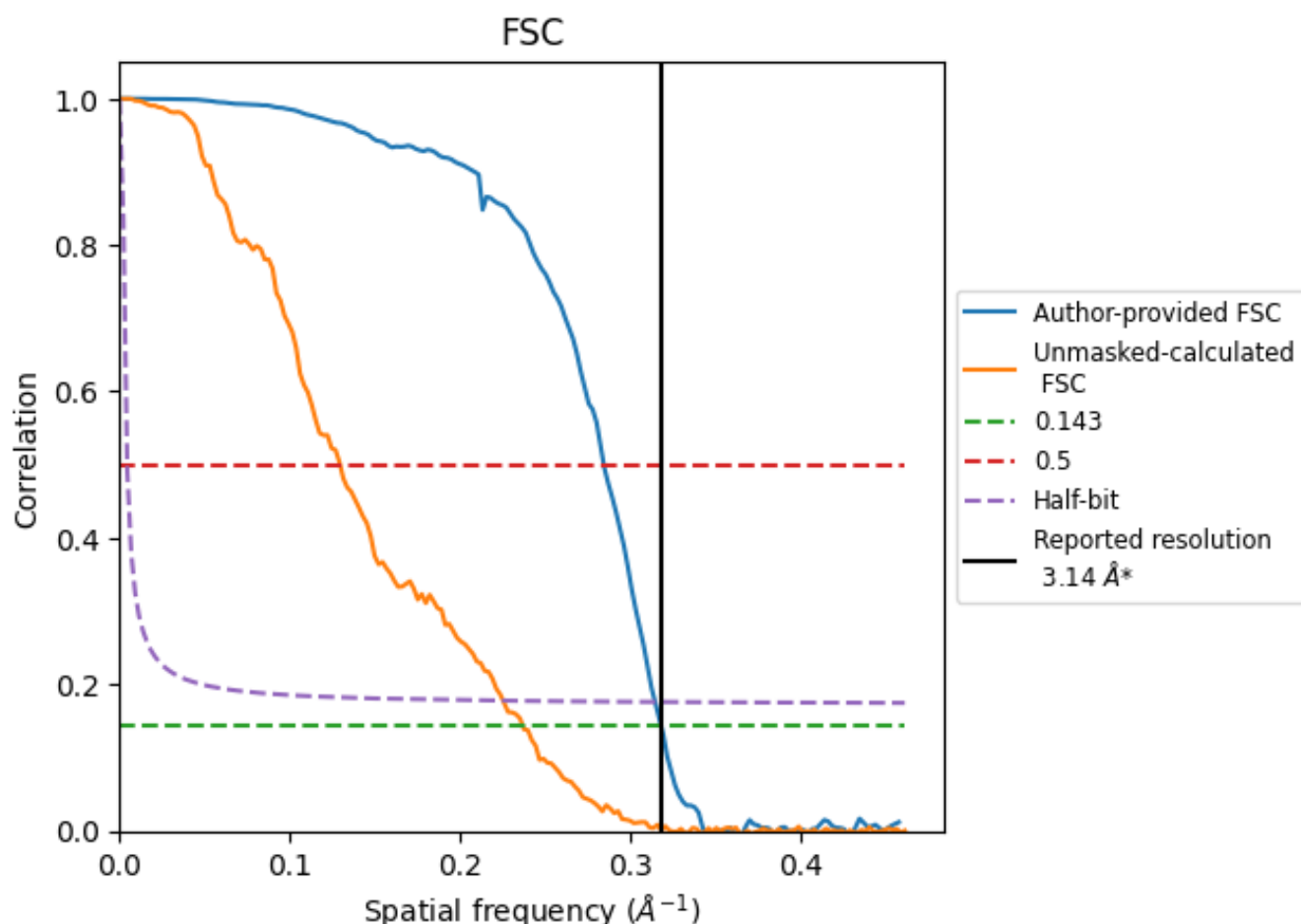


*Reported resolution corresponds to spatial frequency of 0.318 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.318 Å⁻¹

8.2 Resolution estimates [i](#)

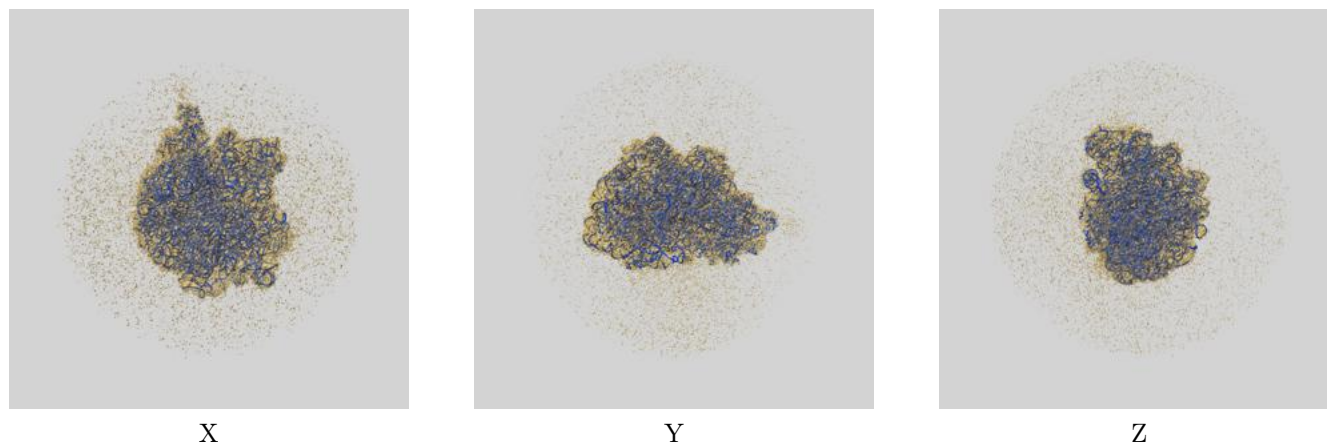
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.14	-	-
Author-provided FSC curve	3.14	3.51	3.18
Unmasked-calculated*	4.22	7.72	4.43

*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 4.22 differs from the reported value 3.14 by more than 10 %

9 Map-model fit [i](#)

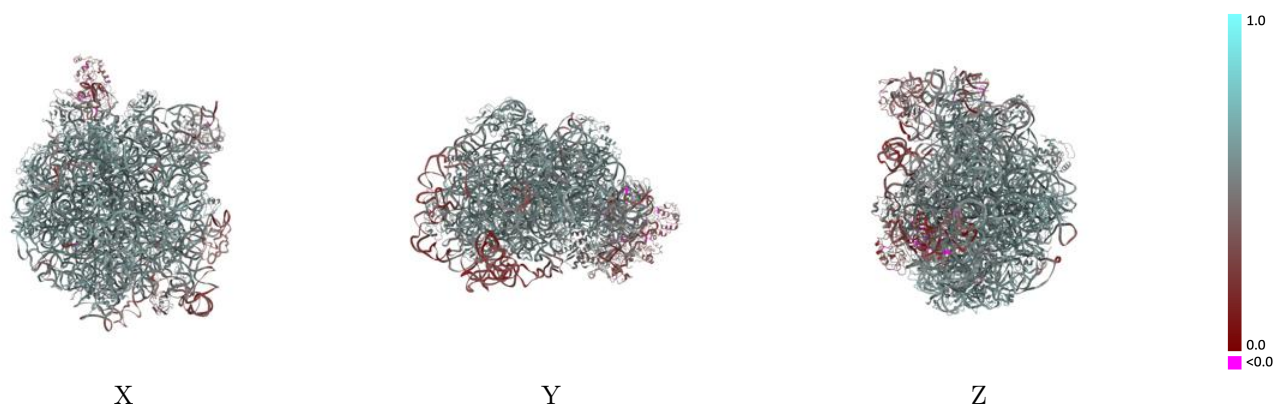
This section contains information regarding the fit between EMDB map EMD-43294 and PDB model 8VK0. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



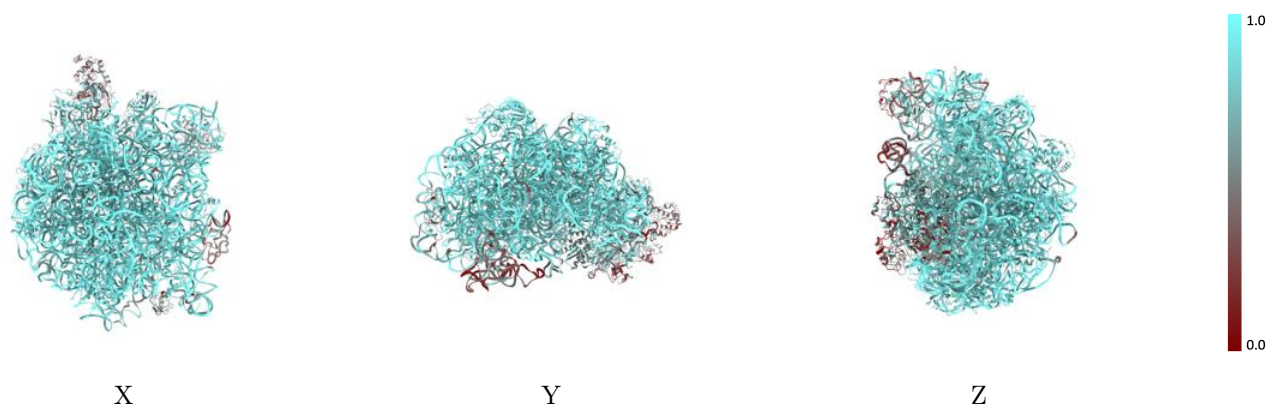
The images above show the 3D surface view of the map at the recommended contour level 0.19 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



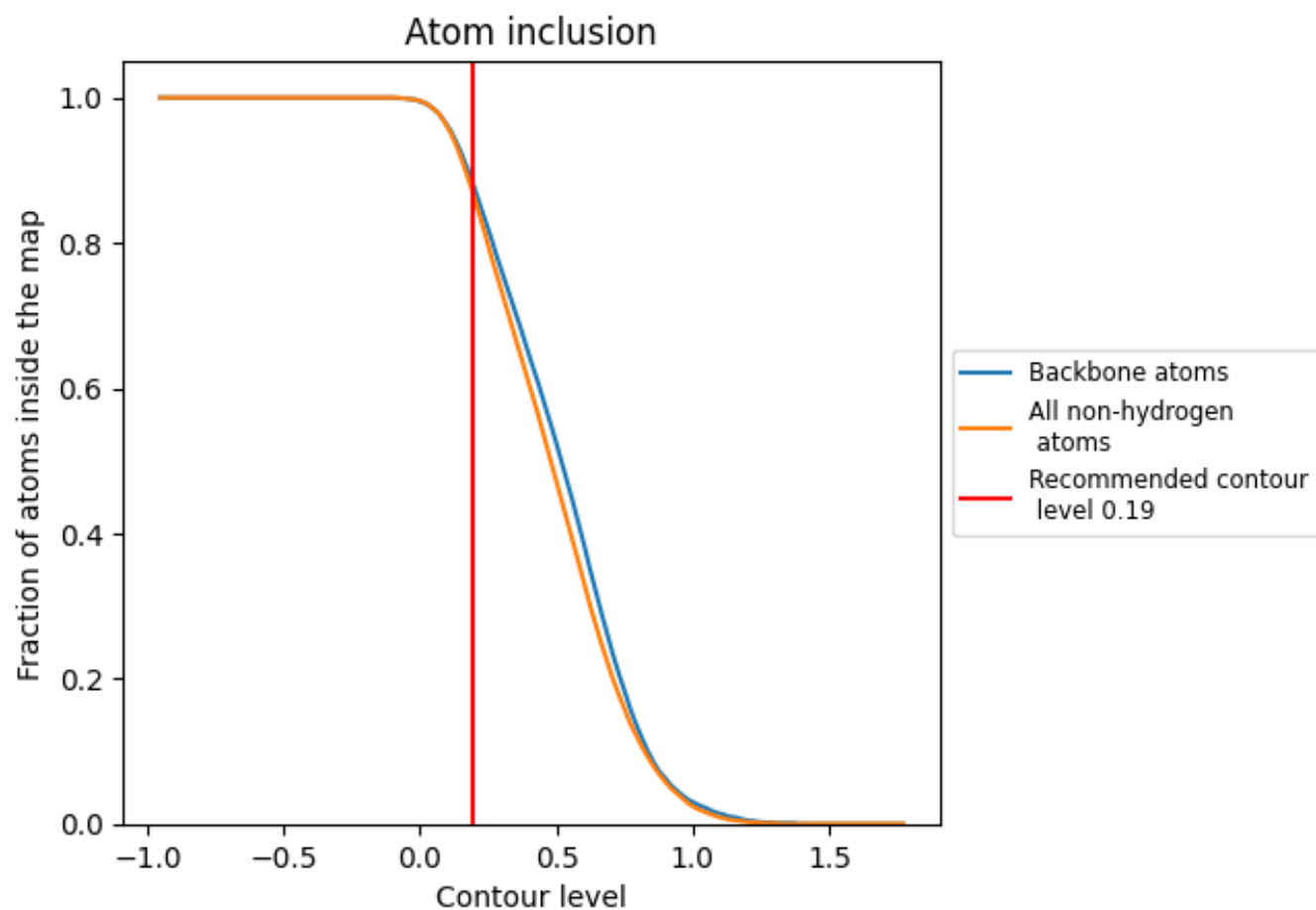
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.19).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 87% 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 (0.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8740	 0.5190
2	 0.9410	 0.5870
3	 0.8660	 0.5910
4	 0.6210	 0.4740
A	 0.9060	 0.5190
B	 0.9180	 0.4820
C	 0.9240	 0.5820
D	 0.9270	 0.5810
E	 0.9000	 0.5690
F	 0.6140	 0.3960
G	 0.7870	 0.4960
H	 0.5930	 0.4280
I	 0.3830	 0.2960
J	 0.3570	 0.2730
K	 0.9350	 0.5860
L	 0.8990	 0.5700
M	 0.9170	 0.5720
N	 0.8540	 0.5740
O	 0.9300	 0.5840
P	 0.7640	 0.4290
Q	 0.8660	 0.5520
R	 0.9370	 0.5890
S	 0.9310	 0.5870
T	 0.9240	 0.5810
U	 0.9120	 0.5700
V	 0.8560	 0.5250
W	 0.7330	 0.5330
X	 0.9190	 0.5790
Y	 0.9230	 0.5720
Z	 0.8900	 0.5520
b	 0.9030	 0.5800
c	 0.9090	 0.5780
d	 0.9230	 0.5910
e	 0.9190	 0.5970
f	 0.8570	 0.5790
g	 0.3360	 0.3560

