



Full wwPDB EM Validation Report ⓘ

Aug 17, 2026 – 09:30 AM EDT

PDB ID : 9Q44 / pdb_00009q44
EMDB ID : EMD-72220
Title : Pseudomonas aeruginosa 50S ribosome bound to RsfS (L1 stalk in 'out' conformation and missing uL1 and tRNA)
Authors : Findlay, J.L.; Kanik, M.; Gauvin, C.C.; Franklin, M.J.; Lawrence, C.M.
Deposited on : 2025-08-19
Resolution : 2.29 Å (reported)
Based on initial models : ., 7UNW

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:

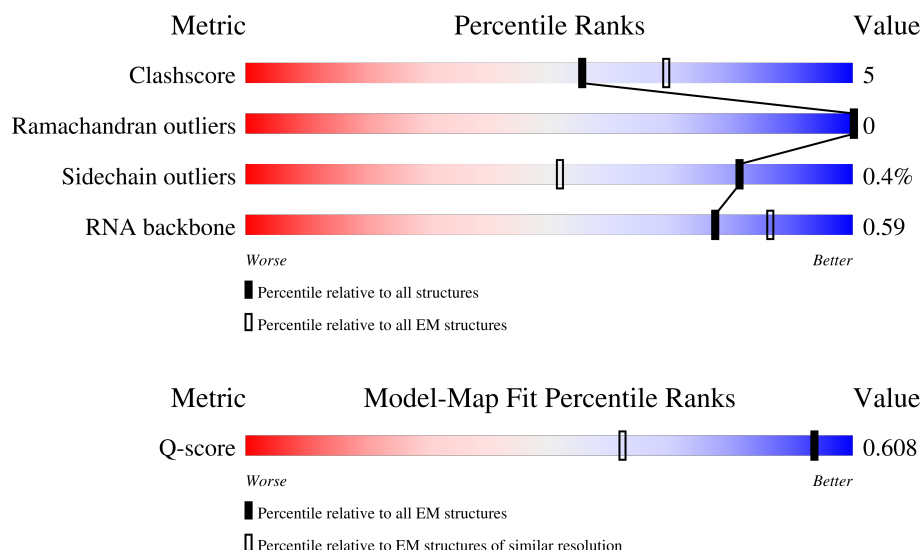
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

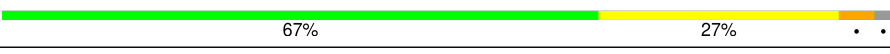
The reported resolution of this entry is 2.29 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	3699 (1.79 - 2.79)

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	A	2892	
2	B	121	
3	D	273	

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Mol	Chain	Length	Quality of chain
4	E	211	
5	F	200	
6	G	179	
7	H	177	
8	I	148	
9	L	142	
10	M	122	
11	N	144	
12	O	137	
13	P	129	
14	Q	116	
15	R	116	
16	S	118	
17	T	103	
18	U	110	
19	V	99	
20	W	104	
21	X	204	
22	Y	85	
23	Z	78	
24	1	63	
25	2	58	
26	4	60	
27	5	51	
28	6	44	

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Mol	Chain	Length	Quality of chain
29	7	64	84% 14%
30	8	38	84% 16%
31	9	118	72% 16% 12%
32	J	166	6% 57% 10% 33%
33	K	143	85% 15%

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 96632 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2837	Total	C	N	O	P	0	0
			60895	27173	11178	19708	2836		

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	119	Total	C	N	O	P	0	0
			2535	1132	452	832	119		

- Molecule 3 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	272	Total	C	N	O	S	0	0
			2072	1276	426	364	6		

- Molecule 4 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	208	Total	C	N	O	S	0	0
			1564	968	298	293	5		

- Molecule 5 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	200	Total	C	N	O	S	0	0
			1521	955	283	280	3		

- Molecule 6 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	179	Total	C	N	O	S	0	0
			1435	914	256	260	5		

- Molecule 7 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	174	Total	C	N	O	S	0	0
			1314	828	242	242	2		

- Molecule 8 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	115	Total	C	N	O	S	0	0
			858	539	152	166	1		

- Molecule 9 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	142	Total	C	N	O	S	0	0
			1130	718	206	202	4		

- Molecule 10 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 11 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	144	Total	C	N	O	S	0	0
			1066	654	215	194	3		

- Molecule 12 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	137	Total	C	N	O	S	0	0
			1085	689	211	181	4		

- Molecule 13 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	119	Total	C	N	O	S	0	0
			952	595	191	161	5		

- Molecule 14 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	115	Total	C	N	O	S	0	0
			881	544	174	161	2		

- Molecule 15 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	114	Total	C	N	O	S	0	0
			901	567	171	162	1		

- Molecule 16 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	117	Total	C	N	O	S	0	0
			936	592	196	148			

- Molecule 17 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	103	Total	C	N	O	S	0	0
			822	521	156	143	2		

- Molecule 18 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	110	Total	C	N	O	S	0	0
			833	515	161	153	4		

- Molecule 19 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	V	94	Total	C	N	O	S	0	0
			739	472	134	132	1		

- Molecule 20 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	95	Total	C	N	O	S	0	0
			738	466	142	129	1		

- Molecule 21 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	X	190	Total	C	N	O	S	0	0
			1445	915	262	265	3		

- Molecule 22 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	77	Total	C	N	O		0	0
			581	367	112	102			

- Molecule 23 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	77	Total	C	N	O	S	0	0
			630	391	134	103	2		

- Molecule 24 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1	61	Total	C	N	O	S	0	0
			490	301	96	91	2		

- Molecule 25 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	2	56	Total	C	N	O	S	0	0
			440	275	86	77	2		

- Molecule 26 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	4	54	Total	C	N	O	S	0	0
			431	258	91	81	1		

- Molecule 27 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	5	51	Total	C	N	O	S	0	0
			426	272	78	75	1		

- Molecule 28 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	6	44	Total	C	N	O	S	0	0
			365	222	87	54	2		

- Molecule 29 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	7	63	Total	C	N	O	S	0	0
			506	314	108	81	3		

- Molecule 30 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	8	38	Total	C	N	O	S	0	0
			307	186	69	48	4		

- Molecule 31 is a protein called Ribosomal silencing factor RsfS.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	9	104	Total	C	N	O	S	0	0
			804	504	135	162	3		

- Molecule 32 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	J	111	Total	C	N	O	S	0	0
			840	533	151	155	1		

- Molecule 33 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	K	143	Total	C	N	O	S	0	0
			1046	655	186	201	4		

- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
34	A	195	Total	Mg	0
			195	195	
34	B	3	Total	Mg	0
			3	3	
34	D	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
34	E	1	Total 1	Mg 1	0
34	S	1	Total 1	Mg 1	0
34	4	1	Total 1	Mg 1	0

- Molecule 35 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
35	8	1	Total 1	Zn 1	0

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		AltConf
36	A	4039	Total 4039	O 4039	0
36	B	76	Total 76	O 76	0
36	D	91	Total 91	O 91	0
36	E	81	Total 81	O 81	0
36	F	49	Total 49	O 49	0
36	G	10	Total 10	O 10	0
36	H	4	Total 4	O 4	0
36	I	1	Total 1	O 1	0
36	L	31	Total 31	O 31	0
36	M	20	Total 20	O 20	0
36	N	64	Total 64	O 64	0
36	O	36	Total 36	O 36	0
36	P	32	Total 32	O 32	0

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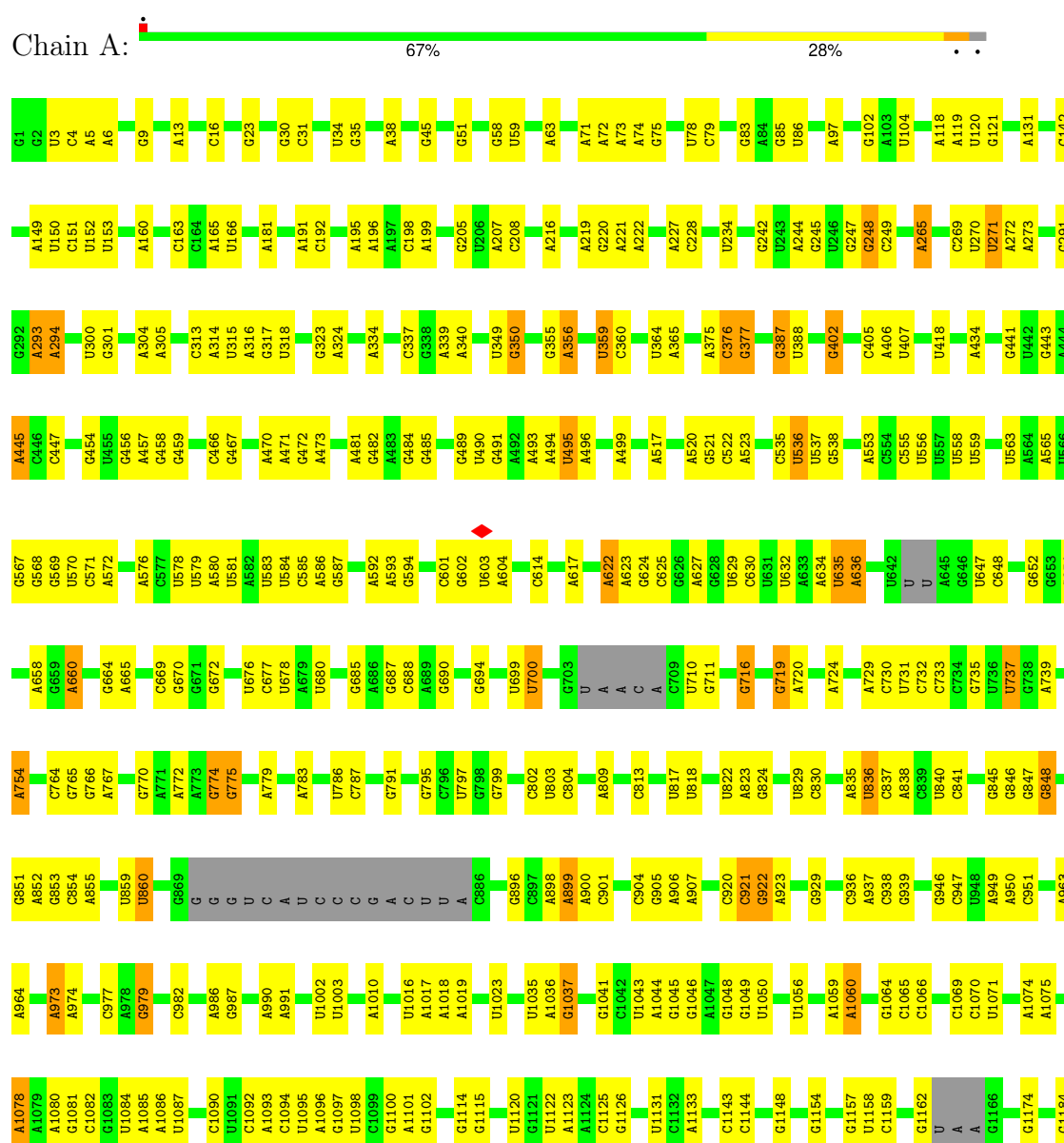
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Mol	Chain	Residues	Atoms		AltConf
36	Q	7	Total 7	O 7	0
36	R	26	Total 26	O 26	0
36	S	46	Total 46	O 46	0
36	T	35	Total 35	O 35	0
36	U	39	Total 39	O 39	0
36	V	30	Total 30	O 30	0
36	W	9	Total 9	O 9	0
36	X	22	Total 22	O 22	0
36	Y	25	Total 25	O 25	0
36	Z	21	Total 21	O 21	0
36	1	4	Total 4	O 4	0
36	2	18	Total 18	O 18	0
36	4	32	Total 32	O 32	0
36	5	3	Total 3	O 3	0
36	6	19	Total 19	O 19	0
36	7	24	Total 24	O 24	0
36	8	9	Total 9	O 9	0

3 Residue-property plots

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

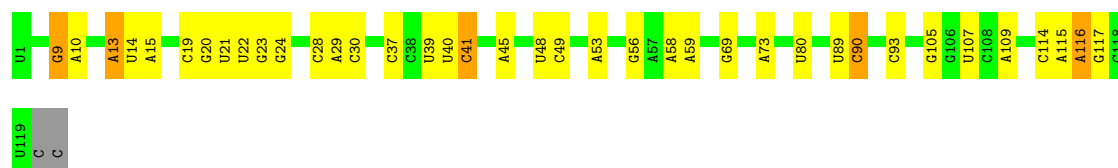
• Molecule 1: 23S rRNA



A2768	U2624	C2306	G2191	A2113	U2013	A	G1461	A1352	U1185
U2771	G2625	A2307	C2195	G2114	A2017	C	G1469	C1357	U1186
A2775	A2626	A2308	G2198	G2115	A2018	G	G1496	G1358	C1187
C2776	G2627	A2309	A2198	U2118	G2019	G1009	A1495	A1365	A1192
C2633	C2634	A2312	C2201	U2119	A2020	U1911	A1966	U1366	G1193
U2634	G2635	A2315	A2212	G2120	G2025	C1912	G1511	G1372	G1199
G2636	A2637	A2316	U2220	A2121	U2026	U1913	A1515	A1374	G1223
G2637	C2638	A2317	G2221	A2122	U2030	U1915	G1656	U1374	G1237
U2638	A2639	A2318	G2225	C2124	U2038	G1917	A1658	A1379	G1237
U2643	G2640	A2323	G2226	G2128	U2042	U1918	G1684	U1380	A1240
A2644	A2645	G2326	G2227	A2129	C2043	U1923	G1672	A1381	U1241
C2645	A2646	C2327	A2228	G2130	G2044	A1925	C1673	A1382	U1242
G2648	U2649	U2330	A2229	G2131	A2047	U1926	A1674	U1392	G1243
C2652	U2650	U2331	U2230	U2137	G2048	U1933	G1689	U1393	U1250
A2653	G2651	U2332	U2231	C2138	A2049	C1934	G1692	U1394	G1251
G2654	C2652	U2333	U2232	G2139	C2050	U1934	G1693	U1395	A1252
U2655	G2653	C2334	G2233	C2140	C2051	C1934	U1694	G1403	A1256
U2656	G2654	U2335	A2234	G2141	C2052	U1942	G1708	G1404	C1257
A2659	A2660	G2336	G2238	U2142	C2053	U1950	G1709	A1405	G1258
G2667	U2661	C2337	C2245	G2143	G2056	G1951	G1710	A1406	A1259
U2674	G2662	A2341	A2246	G2144	U2061	C1952	G1711	U1407	G1265
G2675	U2663	C2346	A2247	G2145	C2060	A1957	G1712	A1414	C1276
U2676	A2664	A2347	A2248	C2146	U2062	U1958	U1717	C1415	A1277
U2677	G2665	G2348	U2258	C2147	U2066	G1959	C1722	G1416	C1284
A2685	C2666	C2349	G2259	C2148	C2066	U1971	G1723	G1418	A1287
G2686	U2667	A2351	A2260	C2149	U2067	U1978	U1724	A1419	A1288
G2701	C2668	G2352	A2261	U2150	C2066	G1979	G1732	A1420	A1289
C2710	U2669	C2358	G2266	C2151	U2073	U1980	G1736	G1422	G1296
U2711	G2670	U2359	G2269	C2152	U2074	C1986	G1740	G1423	U1303
A2712	A2671	G2360	U2270	U2153	U2079	G1989	G1743	U1434	G1304
U2713	C2672	A2361	A2271	U2154	G2080	U1997	C1747	U1435	A1308
G2719	G2673	G2362	G2272	A2158	U2086	U1998	G1751	G1439	U1316
A2720	C2674	A2365	A2274	U2159	U2095	G1999	G1757	U1447	U1339
C2731	G2675	G2366	U2278	C2161	U2096	A2000	A1598	A1340	A1341
A2735	U2676	U2367	G2279	U2162	G2097	A2001	A1599	C1344	C1344
U2871	G2677	G2370	U2283	U2163	U2098	A2002	A1600	G1345	G1345
U2872	A2740	C2371	U2284	U2164	U2100	A2006	A1608	G1452	A1346
G2873	U2743	U2372	U2285	U2165	A2101	A2007	G1621	G1347	G1347
U2885	A2744	G2376	U2292	U2166	A2102	A2008	A1622	G1348	G1348
A2890	G2750	U2377	C2293	U2167	G2103	U2009	G1623	U1350	U1351
U2899	A2751	G2378	G2294	U2168	A2104	G2011	A1624		
A2866	G2752	A2379	G2295	U2169	U2105	C2012			
C2867	U2753	U2388	A2298	U2170	A2106				
U2871	U2760	U	U2299	A2171	G2107				
U2872	A2765	C2380	G2300	U2172	G2108				
G2873	U2766	U2383	C2304	U2173					
U2885	G2767	A2394	G2305	U2174					
A2890				U2175					
U				U2176					
A				A2177					

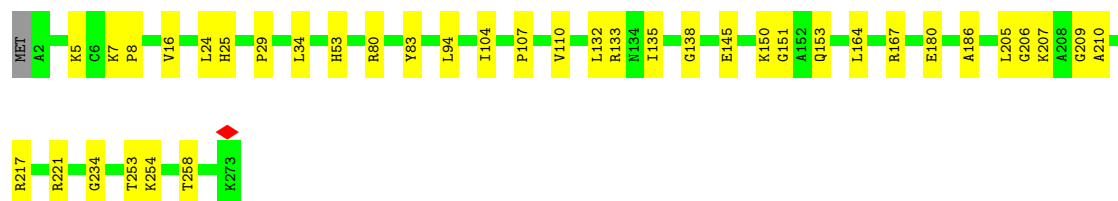
• Molecule 2: 5S rRNA

Chain B: 



- Molecule 3: Large ribosomal subunit protein uL2

Chain D: 



- Molecule 4: Large ribosomal subunit protein uL3

Chain E: 



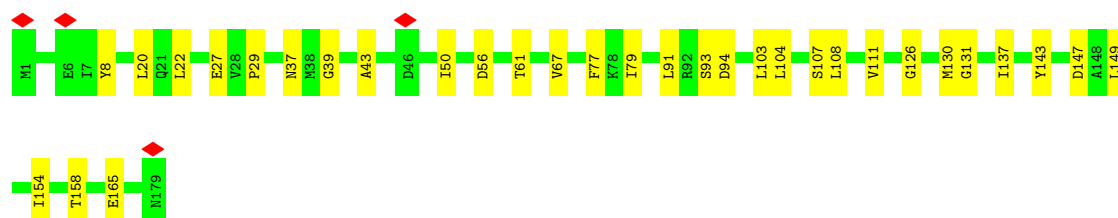
- Molecule 5: Large ribosomal subunit protein uL4

Chain F: 



- Molecule 6: Large ribosomal subunit protein uL5

Chain G: 

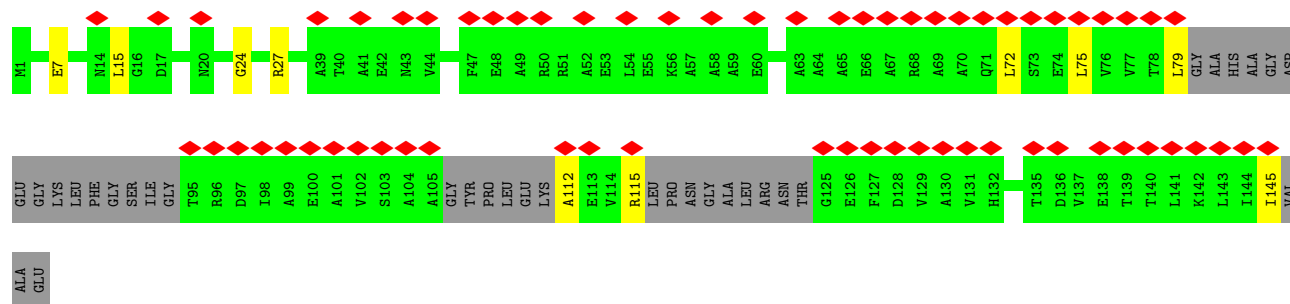
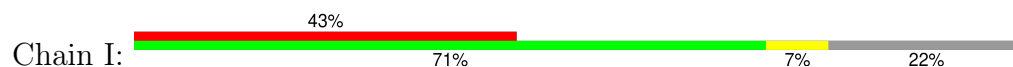


- Molecule 7: Large ribosomal subunit protein uL6

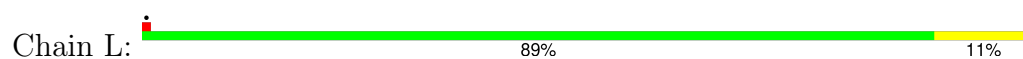
Chain H: 



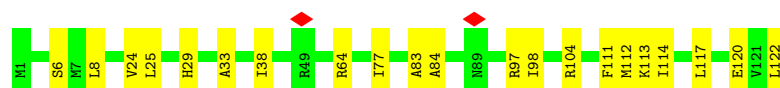
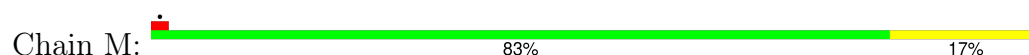
- Molecule 8: Large ribosomal subunit protein bL9



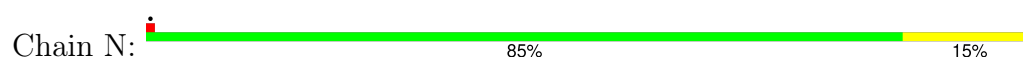
- Molecule 9: Large ribosomal subunit protein uL13



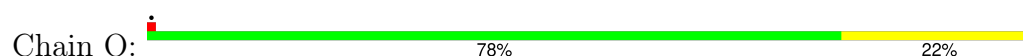
- Molecule 10: Large ribosomal subunit protein uL14



- Molecule 11: Large ribosomal subunit protein uL15



- Molecule 12: Large ribosomal subunit protein uL16



- Molecule 13: Large ribosomal subunit protein bL17

Chain P:  81% 12% 8%



- Molecule 14: Large ribosomal subunit protein uL18

Chain Q:  80% 19% .



- Molecule 15: Large ribosomal subunit protein bL19

Chain R:  5% 84% 15% .



- Molecule 16: Large ribosomal subunit protein bL20

Chain S:  86% 13% .



- Molecule 17: Large ribosomal subunit protein bL21

Chain T:  85% 15%



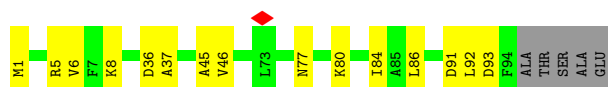
- Molecule 18: Large ribosomal subunit protein uL22

Chain U:  88% 12%



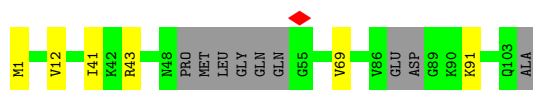
- Molecule 19: Large ribosomal subunit protein uL23

Chain V:  80% 15% 5%



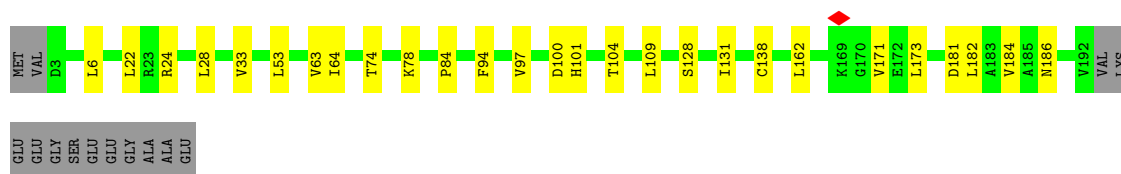
- Molecule 20: Large ribosomal subunit protein uL24

Chain W:  86% 6% 9%



- Molecule 21: Large ribosomal subunit protein bL25

Chain X:  80% 13% 7%



- Molecule 22: Large ribosomal subunit protein bL27

Chain Y:  86% 5% 9%



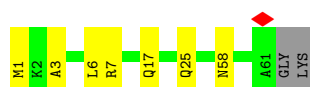
- Molecule 23: Large ribosomal subunit protein bL28

Chain Z:  86% 13% .

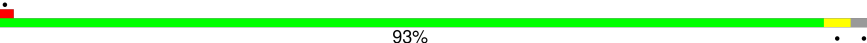


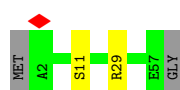
- Molecule 24: Large ribosomal subunit protein uL29

Chain 1:  86% 11% .



- Molecule 25: Large ribosomal subunit protein uL30

Chain 2:  93% . .



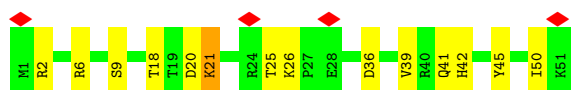
- Molecule 26: Large ribosomal subunit protein bL32

Chain 4:  80% 10% 10%



- Molecule 27: Large ribosomal subunit protein bL33

Chain 5:  8% 73% 25%



- Molecule 28: Large ribosomal subunit protein bL34

Chain 6:  73% 25%



- Molecule 29: Large ribosomal subunit protein bL35

Chain 7:  84% 14%



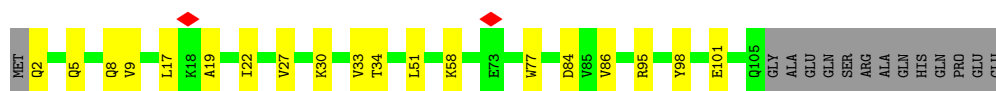
- Molecule 30: Large ribosomal subunit protein bL36A

Chain 8:  84% 16%



- Molecule 31: Ribosomal silencing factor RsfS

Chain 9:  72% 16% 12%



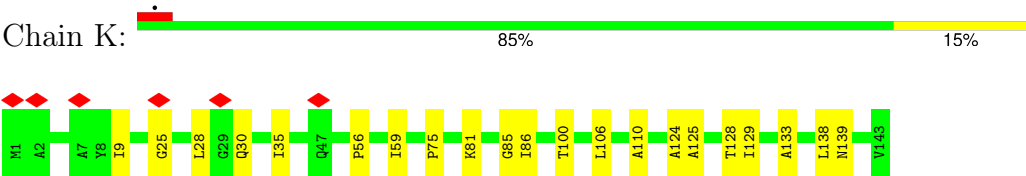
- Molecule 32: Large ribosomal subunit protein uL10

Chain J:  6% 57% 10% 33%



ILE
ASP
VAL
LEU
ALA
SER
LEU
PRO
THR
TYR
ASP
GLU
ALA
VAL
SER
GLN
LEU
MET
SER
VAL
ILE
GLN
GLY
ALA
THR
SER
LYS
LEU
ALA
ARG
THR
LEU
ALA
ALA
ILE
ARG
ASP
GLN
LYS
GLU
ALA
ALA
ALA

● Molecule 33: Large ribosomal subunit protein uL10



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	452165	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54.3	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	36000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	66.579	Depositor
Minimum map value	-43.550	Depositor
Average map value	0.003	Depositor
Map value standard deviation	1.055	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	468.408, 468.408, 468.408	wwPDB
Map dimensions	696, 696, 696	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.673, 0.673, 0.673	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 5MC, 7MG, 6MZ, OMC, 5MU, ZN, OMG, 1MG, OMU, 2MG, 2MA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.23	0/67882	0.26	0/105870
2	B	0.12	0/2833	0.21	0/4413
3	D	0.16	0/2108	0.29	0/2831
4	E	0.17	0/1587	0.31	0/2138
5	F	0.09	0/1541	0.23	0/2075
6	G	0.13	0/1456	0.26	0/1953
7	H	0.10	0/1332	0.22	0/1794
8	I	0.14	0/861	0.30	0/1159
9	L	0.12	0/1156	0.28	0/1559
10	M	0.10	0/947	0.26	0/1268
11	N	0.08	0/1078	0.23	0/1436
12	O	0.08	0/1105	0.21	0/1476
13	P	0.17	0/968	0.36	0/1294
14	Q	0.18	0/888	0.23	0/1183
15	R	0.20	0/910	0.32	0/1218
16	S	0.16	0/946	0.31	0/1257
17	T	0.09	0/835	0.21	0/1117
18	U	0.10	0/837	0.22	0/1114
19	V	0.08	0/749	0.23	0/1002
20	W	0.09	0/743	0.27	0/988
21	X	0.13	0/1468	0.26	0/1987
22	Y	0.13	0/589	0.37	0/782
23	Z	0.15	0/641	0.25	0/854
24	1	0.14	0/491	0.23	0/654
25	2	0.19	0/444	0.27	0/597
26	4	0.09	0/437	0.23	0/583
27	5	0.12	0/433	0.27	0/576
28	6	0.18	0/368	0.36	0/482
29	7	0.15	0/511	0.34	0/668
30	8	0.09	0/308	0.19	0/404
31	9	0.17	0/813	0.35	0/1103
32	J	0.08	0/850	0.22	0/1142

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	K	0.08	0/1061	0.23	0/1435
All	All	0.21	0/99176	0.26	0/148412

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	60895	0	30645	483	0
2	B	2535	0	1283	20	0
3	D	2072	0	2152	26	0
4	E	1564	0	1575	21	0
5	F	1521	0	1581	27	0
6	G	1435	0	1504	21	0
7	H	1314	0	1373	15	0
8	I	858	0	890	6	0
9	L	1130	0	1160	11	0
10	M	938	0	1012	16	0
11	N	1066	0	1112	15	0
12	O	1085	0	1157	21	0
13	P	952	0	996	11	0
14	Q	881	0	920	14	0
15	R	901	0	958	14	0
16	S	936	0	1025	13	0
17	T	822	0	858	11	0
18	U	833	0	897	8	0
19	V	739	0	788	10	0
20	W	738	0	806	4	0
21	X	1445	0	1486	18	0
22	Y	581	0	603	3	0
23	Z	630	0	653	8	0
24	1	490	0	520	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	2	440	0	469	2	0
26	4	431	0	424	6	0
27	5	426	0	457	10	0
28	6	365	0	409	10	0
29	7	506	0	569	11	0
30	8	307	0	342	4	0
31	9	804	0	809	13	0
32	J	840	0	867	10	0
33	K	1046	0	1089	14	0
34	4	1	0	0	0	0
34	A	195	0	0	0	0
34	B	3	0	0	0	0
34	D	1	0	0	0	0
34	E	1	0	0	0	0
34	S	1	0	0	0	0
35	8	1	0	0	0	0
36	1	4	0	0	0	0
36	2	18	0	0	0	0
36	4	32	0	0	1	0
36	5	3	0	0	1	0
36	6	19	0	0	1	0
36	7	24	0	0	1	0
36	8	9	0	0	0	0
36	A	4039	0	0	16	0
36	B	76	0	0	1	0
36	D	91	0	0	1	0
36	E	81	0	0	0	0
36	F	49	0	0	1	0
36	G	10	0	0	0	0
36	H	4	0	0	0	0
36	I	1	0	0	0	0
36	L	31	0	0	0	0
36	M	20	0	0	0	0
36	N	64	0	0	0	0
36	O	36	0	0	0	0
36	P	32	0	0	0	0
36	Q	7	0	0	0	0
36	R	26	0	0	1	0
36	S	46	0	0	2	0
36	T	35	0	0	0	0
36	U	39	0	0	1	0
36	V	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	W	9	0	0	1	0
36	X	22	0	0	0	0
36	Y	25	0	0	0	0
36	Z	21	0	0	1	0
All	All	96632	0	61389	753	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (753) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:C:HO2'	1:A:340:A:H8	1.25	0.81
7:H:16:GLU:HB2	7:H:27:LYS:HB3	1.71	0.72
1:A:1692:G:N7	36:A:3104:HOH:O	2.22	0.72
1:A:558:U:H1'	1:A:2017:6MZ:H9C1	1.73	0.70
1:A:1046:G:O2'	1:A:1093:A:N6	2.25	0.69
7:H:164:TYR:HB2	7:H:167:GLU:HB2	1.73	0.69
1:A:339:A:N1	36:A:3123:HOH:O	2.25	0.68
2:B:41:C:N4	6:G:67:VAL:O	2.26	0.68
33:K:100:THR:HG22	33:K:139:ASN:HB2	1.74	0.68
1:A:291:G:N7	36:A:3138:HOH:O	2.27	0.67
28:6:1:MET:SD	28:6:3:ARG:NH2	2.68	0.67
1:A:920:C:OP2	25:2:29:ARG:NH1	2.25	0.66
1:A:2315:A:H2'	1:A:2316:A:C8	2.31	0.66
33:K:9:ILE:HB	33:K:59:ILE:HB	1.78	0.66
32:J:27:VAL:HG13	32:J:80:THR:HG23	1.77	0.65
1:A:694:G:O2'	1:A:716:G:N2	2.25	0.64
7:H:87:LEU:HB2	7:H:131:ILE:HB	1.81	0.63
1:A:1997:G:N7	36:A:3193:HOH:O	2.31	0.63
1:A:2010:C:H5'	1:A:2604:U:H4'	1.81	0.63
1:A:2292:U:H5''	6:G:131:GLY:HA3	1.80	0.63
1:A:1085:A:H61	33:K:30:GLN:HE22	1.47	0.63
1:A:896:G:H5'	12:O:23:ARG:HB3	1.80	0.62
15:R:95:LYS:NZ	36:R:202:HOH:O	2.31	0.62
1:A:1084:U:H1'	1:A:1087:U:H5	1.64	0.62
1:A:1095:U:H2'	1:A:1096:A:H8	1.63	0.62
1:A:963:A:H5''	17:T:81:LYS:HD2	1.82	0.62
21:X:162:LEU:HD12	21:X:182:LEU:H	1.63	0.62
12:O:67:ARG:NH1	12:O:105:GLU:OE2	2.32	0.62
15:R:101:LEU:HD11	15:R:111:ILE:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:41:GLU:HG3	4:E:47:ARG:HG3	1.82	0.61
12:O:78:PRO:HG2	12:O:81:VAL:HG21	1.82	0.61
5:F:147:ILE:HG23	5:F:186:LEU:HD23	1.82	0.61
26:4:2:ALA:N	36:4:203:HOH:O	2.34	0.61
1:A:2645:C:OP1	7:H:160:LYS:NZ	2.33	0.61
24:1:1:MET:SD	24:1:17:GLN:NE2	2.74	0.61
1:A:2278:U:H2'	1:A:2279:G:C8	2.36	0.60
1:A:896:G:OP1	12:O:24:GLY:N	2.33	0.60
1:A:1788:A:OP2	3:D:150:LYS:NZ	2.34	0.60
1:A:160:A:N3	1:A:2195:C:O2'	2.33	0.60
1:A:459:G:N7	28:6:39:ARG:NH2	2.40	0.60
1:A:1071:U:H4'	33:K:124:ALA:HB1	1.84	0.60
1:A:1834:A:O2'	1:A:1835:A:N7	2.35	0.60
1:A:2835:G:O2'	1:A:2854:G:N2	2.26	0.60
1:A:2293:C:H42	6:G:39:GLY:HA3	1.65	0.59
1:A:688:C:O2'	1:A:724:A:N6	2.35	0.59
33:K:28:LEU:HD12	33:K:35:ILE:HG23	1.84	0.59
1:A:1766:U:OP2	1:A:1771:A:N6	2.31	0.59
3:D:53:HIS:HA	3:D:217:ARG:HB2	1.84	0.59
21:X:128:SER:OG	21:X:186:ASN:OD1	2.20	0.59
1:A:1689:G:N3	36:A:3227:HOH:O	2.32	0.58
1:A:2112:G:H22	1:A:2159:U:H5'	1.68	0.58
1:A:2775:A:H2'	1:A:2776:C:C6	2.38	0.58
1:A:1049:G:H21	33:K:128:THR:HG23	1.69	0.58
1:A:1710:A:N7	1:A:1724:U:O2'	2.33	0.58
1:A:359:U:H5''	1:A:360:C:H5'	1.86	0.58
17:T:14:VAL:HG13	17:T:98:ILE:HG13	1.85	0.58
1:A:1420:A:H2'	1:A:1421:A:C8	2.39	0.57
1:A:1766:U:H5	1:A:1771:A:N7	2.03	0.57
1:A:1587:A:H5''	1:A:1588:A:H5'	1.87	0.57
1:A:2260:A:H2'	1:A:2261:A:C8	2.40	0.57
1:A:5:A:H2'	1:A:6:A:C8	2.40	0.57
31:9:2:GLN:HB3	31:9:5:GLN:HG2	1.87	0.57
1:A:921:C:H4'	1:A:922:G:H5'	1.85	0.57
1:A:1404:C:HO2'	1:A:1577:G:HO2'	1.52	0.57
10:M:25:LEU:HD12	10:M:38:ILE:HG22	1.86	0.57
12:O:122:ALA:HA	12:O:125:LEU:HD12	1.87	0.57
27:5:6:ARG:NH2	27:5:50:ILE:O	2.37	0.57
13:P:79:LEU:HA	13:P:83:LEU:HB2	1.87	0.56
1:A:1237:G:O6	11:N:18:ARG:NH2	2.37	0.56
12:O:76:LYS:HB2	12:O:91:GLU:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:64:ARG:HB2	10:M:83:ALA:HB3	1.87	0.56
1:A:797:U:OP2	11:N:41:ARG:NH2	2.38	0.56
1:A:1060:A:N7	1:A:1086:A:O2'	2.36	0.56
1:A:2162:C:H2'	1:A:2163:A:H8	1.70	0.56
5:F:3:LEU:HD12	5:F:13:VAL:HG11	1.87	0.56
1:A:2140:C:H2'	1:A:2141:G:H8	1.69	0.56
1:A:1018:A:H2'	1:A:1019:A:C8	2.41	0.56
1:A:1056:U:N3	1:A:1059:A:OP2	2.34	0.56
1:A:1284:C:O2'	1:A:1289:A:N1	2.34	0.56
14:Q:20:ARG:HH21	14:Q:45:GLY:HA3	1.71	0.56
1:A:853:G:H2'	1:A:854:C:C6	2.41	0.55
21:X:78:LYS:NZ	21:X:104:THR:O	2.39	0.55
33:K:56:PRO:HD3	33:K:75:PRO:HD3	1.87	0.55
1:A:2775:A:O2'	1:A:2796:A:N3	2.39	0.55
2:B:13:A:N1	2:B:69:G:O2'	2.35	0.55
2:B:15:A:OP2	2:B:69:G:N2	2.33	0.55
7:H:9:VAL:HG13	7:H:73:ASN:HD22	1.71	0.55
18:U:92:ARG:NH1	36:U:205:HOH:O	2.38	0.55
1:A:1821:U:H5''	1:A:1822:2MG:H5'	1.88	0.55
1:A:2406:U:H4'	27:5:18:THR:HG21	1.89	0.55
1:A:59:U:OP2	19:V:77:ASN:ND2	2.40	0.55
1:A:72:A:H61	24:1:58:ASN:HD22	1.52	0.55
3:D:138:GLY:H	3:D:164:LEU:HB3	1.72	0.55
27:5:2:ARG:HB3	27:5:20:ASP:HB2	1.89	0.55
1:A:1373:C:H2'	1:A:1374:A:C8	2.42	0.55
1:A:1419:G:H2'	1:A:1420:A:C8	2.41	0.55
19:V:5:ARG:NH2	19:V:36:ASP:OD2	2.39	0.55
21:X:53:LEU:HD21	21:X:64:ILE:HD13	1.88	0.55
1:A:219:A:N3	1:A:234:U:O2'	2.37	0.55
1:A:1926:5MU:OP1	1:A:2591:U:O2'	2.23	0.55
1:A:2805:C:OP2	13:P:42:LYS:HE2	2.06	0.55
1:A:1074:A:N3	1:A:1095:U:O2'	2.32	0.55
1:A:1788:A:OP2	3:D:153:GLN:NE2	2.29	0.55
10:M:120:GLU:OE1	15:R:66:SER:OG	2.25	0.54
1:A:567:G:O2'	1:A:1241:A:OP1	2.26	0.54
1:A:1456:A:H2'	1:A:1457:A:C8	2.42	0.54
1:A:907:A:N3	2:B:80:U:O2'	2.39	0.54
1:A:571:C:H2'	1:A:572:A:C8	2.42	0.54
1:A:2102:G:H2'	1:A:2104:A:N7	2.23	0.54
1:A:2498:U:H5''	4:E:128:ARG:HG3	1.90	0.54
1:A:1406:A:O2'	1:A:1408:G:N7	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2534:A:H2'	1:A:2535:U:C6	2.43	0.54
3:D:132:LEU:HA	3:D:135:ILE:HD12	1.90	0.54
1:A:592:A:O2'	1:A:594:G:O2'	2.21	0.54
1:A:2096:U:H2'	1:A:2097:G:C8	2.42	0.54
1:A:2300:C:O4'	6:G:37:ASN:ND2	2.40	0.54
20:W:43:ARG:NH2	36:W:201:HOH:O	2.41	0.54
1:A:2230:U:H2'	1:A:2231:U:C6	2.42	0.54
10:M:98:ILE:HD13	10:M:114:ILE:HG23	1.90	0.54
1:A:570:U:H2'	1:A:571:C:C6	2.43	0.54
1:A:733:C:O2'	1:A:1649:G:OP1	2.24	0.54
1:A:2172:U:H2'	1:A:2173:G:H8	1.73	0.53
1:A:2245:C:O2'	1:A:2414:C:OP2	2.25	0.53
12:O:34:LEU:HD13	12:O:118:PHE:HB3	1.90	0.53
1:A:78:U:H2'	1:A:79:C:C6	2.44	0.53
13:P:54:LEU:HD21	13:P:65:LEU:HB3	1.90	0.53
1:A:848:G:O2'	1:A:905:G:O6	2.24	0.53
1:A:1783:U:H2'	1:A:1784:C:C6	2.43	0.53
1:A:2061:U:H2'	1:A:2062:U:C6	2.44	0.53
8:I:79:LEU:HD21	8:I:145:ILE:HG12	1.90	0.53
1:A:786:U:H2'	1:A:787:C:C6	2.44	0.53
1:A:632:U:O2'	1:A:634:A:N7	2.40	0.53
1:A:1453:U:O3'	1:A:1536:G:O2'	2.27	0.53
1:A:677:C:H5''	28:6:2:LYS:HE2	1.90	0.53
1:A:244:A:H5''	11:N:67:VAL:HG11	1.91	0.53
1:A:680:U:O2'	1:A:770:G:OP1	2.25	0.53
1:A:764:C:O2'	1:A:767:A:N3	2.41	0.53
1:A:2103:G:N2	1:A:2149:A:OP2	2.41	0.53
1:A:2019:G:O2'	4:E:150:GLN:NE2	2.42	0.52
1:A:2052:C:H2'	1:A:2053:C:H6	1.74	0.52
21:X:74:THR:HG22	21:X:97:VAL:HB	1.90	0.52
1:A:823:A:H2'	1:A:824:G:C8	2.44	0.52
9:L:18:VAL:HG11	9:L:28:LEU:HD11	1.92	0.52
1:A:937:A:H2'	1:A:938:C:C6	2.45	0.52
1:A:1352:A:OP1	23:Z:3:ARG:NH1	2.38	0.52
1:A:754:A:H5'	3:D:209:GLY:HA2	1.91	0.52
1:A:2605:G:H21	4:E:155:VAL:HG21	1.74	0.52
6:G:93:SER:OG	6:G:94:ASP:N	2.42	0.52
7:H:28:GLY:HA3	7:H:79:VAL:HB	1.91	0.52
10:M:77:ILE:HG12	15:R:73:ARG:HD2	1.92	0.52
12:O:54:LEU:HD12	12:O:117:ALA:HB1	1.91	0.52
27:5:41:GLN:NE2	36:5:101:HOH:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:6:25:LYS:NZ	36:6:101:HOH:O	2.43	0.52
31:9:34:THR:HG21	31:9:86:VAL:HG23	1.91	0.52
1:A:899:A:H2'	1:A:900:A:C8	2.45	0.52
6:G:103:LEU:HD12	6:G:107:SER:HB2	1.92	0.52
14:Q:82:LYS:HD2	14:Q:113:GLY:HA3	1.92	0.52
21:X:131:ILE:HD11	21:X:184:VAL:HG22	1.92	0.52
36:B:305:HOH:O	21:X:24:ARG:NH2	2.42	0.52
16:S:16:LYS:NZ	36:S:303:HOH:O	2.43	0.52
7:H:42:GLU:HG2	7:H:55:ARG:HD3	1.91	0.51
9:L:31:GLU:OE2	9:L:35:ARG:NE	2.42	0.51
1:A:1046:G:N1	1:A:1092:C:OP2	2.31	0.51
4:E:156:PHE:HB3	9:L:81:PRO:HG3	1.92	0.51
18:U:82:LEU:HB2	18:U:98:LYS:HB2	1.91	0.51
1:A:441:G:N1	1:A:445:A:OP2	2.37	0.51
1:A:2585:A:H5''	3:D:234:GLY:HA3	1.93	0.51
1:A:5:A:H2'	1:A:6:A:H8	1.76	0.51
17:T:6:VAL:HG22	17:T:11:GLN:HG2	1.91	0.51
29:7:53:ASP:OD1	29:7:56:ARG:NH2	2.43	0.51
1:A:247:G:H4'	1:A:377:G:C5	2.45	0.51
1:A:1085:A:N6	33:K:30:GLN:HE22	2.09	0.51
1:A:2633:C:OP2	1:A:2719:G:O2'	2.29	0.51
6:G:20:LEU:HD13	6:G:165:GLU:HG2	1.92	0.51
23:Z:13:VAL:HG23	23:Z:29:PHE:HB2	1.91	0.51
1:A:265:A:N1	1:A:418:U:O2'	2.44	0.51
1:A:2140:C:H2'	1:A:2141:G:C8	2.46	0.51
1:A:2220:U:H2'	1:A:2221:G:C8	2.45	0.51
21:X:181:ASP:OD1	21:X:181:ASP:N	2.43	0.51
1:A:300:U:H2'	1:A:301:G:O4'	2.10	0.51
1:A:629:U:H2'	1:A:630:C:C6	2.46	0.51
1:A:1043:U:O4	1:A:1044:A:N6	2.44	0.51
1:A:1044:A:H2'	1:A:1045:G:C8	2.46	0.51
1:A:1434:U:O2'	1:A:1534:A:N3	2.38	0.51
1:A:1783:U:H2'	1:A:1784:C:H6	1.76	0.51
1:A:2162:C:H2'	1:A:2163:A:C8	2.45	0.51
1:A:2432:2MG:OP1	5:F:68:ARG:NH1	2.42	0.51
11:N:78:ARG:HB2	11:N:81:GLU:HG3	1.93	0.51
1:A:1348:G:H2'	1:A:1349:C:C6	2.45	0.51
1:A:1373:C:H2'	1:A:1374:A:H8	1.76	0.51
5:F:17:THR:OG1	5:F:200:GLY:O	2.29	0.51
1:A:1185:U:H2'	1:A:1186:U:C6	2.45	0.51
1:A:2058:A:H2'	1:A:2059:C:C6	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2711:U:OP1	4:E:123:LYS:NZ	2.44	0.51
1:A:2821:G:H2'	1:A:2866:A:H61	1.75	0.51
10:M:122:LEU:HD13	15:R:71:VAL:HG11	1.93	0.51
20:W:1:MET:HE3	20:W:91:LYS:HE3	1.93	0.51
1:A:2114:G:N2	1:A:2149:A:O2'	2.44	0.50
18:U:4:ALA:HB2	18:U:106:LYS:HG2	1.93	0.50
19:V:1:MET:HB3	19:V:5:ARG:HB3	1.93	0.50
1:A:191:A:H2'	1:A:192:C:C6	2.47	0.50
1:A:1064:G:H2'	1:A:1065:C:C6	2.46	0.50
1:A:2330:U:O2'	1:A:2360:A:O2'	2.26	0.50
29:7:41:ARG:NH1	36:7:105:HOH:O	2.44	0.50
1:A:836:U:H5	1:A:923:A:N7	2.09	0.50
1:A:456:G:OP1	28:6:12:ARG:NH2	2.44	0.50
1:A:1095:U:H2'	1:A:1096:A:C8	2.45	0.50
1:A:1781:A:H2'	1:A:1782:C:C6	2.46	0.50
36:A:6877:HOH:O	14:Q:14:LYS:CD	2.59	0.50
1:A:2554:G:H2'	1:A:2555:U:C6	2.46	0.50
1:A:2602:U:H1'	26:4:4:GLN:HB3	1.94	0.50
4:E:36:THR:HG22	4:E:74:VAL:HG21	1.94	0.50
15:R:89:ARG:NH2	15:R:111:ILE:O	2.35	0.50
31:9:33:VAL:HG12	31:9:34:THR:HG23	1.93	0.50
1:A:405:C:H2'	1:A:406:A:C8	2.46	0.50
6:G:61:THR:HB	6:G:91:LEU:HD21	1.93	0.50
1:A:2114:G:H2'	1:A:2115:G:H8	1.77	0.50
1:A:2283:U:O2'	1:A:2307:A:N6	2.44	0.50
8:I:7:GLU:HA	8:I:15:LEU:HD12	1.94	0.50
8:I:72:LEU:HA	8:I:75:LEU:HD23	1.94	0.50
1:A:293:A:N3	1:A:313:C:O2'	2.41	0.50
12:O:35:LYS:NZ	21:X:84:PRO:O	2.34	0.50
30:8:2:LYS:HG2	30:8:4:ARG:HD2	1.94	0.50
1:A:700:U:H3	1:A:711:G:H1	1.60	0.50
1:A:1392:U:H2'	1:A:1393:U:C6	2.47	0.50
1:A:1434:U:H2'	1:A:1435:U:C6	2.46	0.50
7:H:121:ILE:HD11	7:H:140:LEU:HG	1.94	0.50
19:V:6:VAL:HG23	19:V:45:ALA:HA	1.94	0.50
1:A:672:G:H5'	28:6:26:ASN:CG	2.37	0.49
1:A:2578:C:H2'	1:A:2579:G:C8	2.46	0.49
1:A:625:C:O2'	1:A:629:U:OP1	2.30	0.49
1:A:2103:G:H2'	1:A:2104:A:N7	2.27	0.49
1:A:2582:G:N2	1:A:2585:A:OP2	2.34	0.49
1:A:2846:G:H2'	1:A:2847:A:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:63:LYS:HD3	12:O:65:TRP:CZ2	2.47	0.49
1:A:729:A:H1'	1:A:730:C:H5	1.77	0.49
1:A:2517:A:N6	7:H:156:PRO:HG3	2.26	0.49
5:F:97:LYS:NZ	36:F:311:HOH:O	2.43	0.49
1:A:1065:C:H2'	1:A:1066:C:C6	2.47	0.49
8:I:112:ALA:O	8:I:115:ARG:NH1	2.44	0.49
1:A:658:A:H2'	1:A:660:A:H62	1.77	0.49
1:A:803:U:H2'	1:A:804:C:C6	2.47	0.49
1:A:2001:A:H2'	1:A:2002:A:C8	2.47	0.49
2:B:28:C:OP1	14:Q:32:SER:OG	2.28	0.49
31:9:19:ALA:HB3	31:9:22:ILE:HD11	1.93	0.49
1:A:491:G:N1	1:A:494:A:OP2	2.41	0.49
1:A:1186:U:H2'	1:A:1187:C:C6	2.46	0.49
27:5:36:ASP:HB3	27:5:39:VAL:HG22	1.95	0.49
9:L:49:ASP:OD1	9:L:121:LYS:NZ	2.45	0.49
6:G:77:PHE:HB2	6:G:79:ILE:HG13	1.93	0.49
1:A:1404:C:O2'	1:A:1577:G:O2'	2.26	0.49
1:A:2183:C:H2'	1:A:2184:U:C6	2.48	0.49
1:A:2379:A:H5'	29:7:27:PHE:CD2	2.47	0.49
36:A:6877:HOH:O	14:Q:14:LYS:HD3	2.13	0.49
6:G:111:VAL:HG22	6:G:137:ILE:HG21	1.94	0.49
1:A:1010:A:N1	1:A:1131:U:O2'	2.44	0.49
1:A:1018:A:N6	1:A:1115:G:H2'	2.28	0.49
1:A:2834:U:H2'	1:A:2835:G:O4'	2.13	0.49
1:A:1097:G:H4'	32:J:78:GLY:C	2.38	0.48
32:J:45:ALA:HB1	32:J:50:VAL:HB	1.94	0.48
32:J:70:ASP:OD1	32:J:73:ASN:ND2	2.46	0.48
1:A:837:C:H2'	1:A:838:A:C8	2.49	0.48
1:A:1036:A:OP2	32:J:62:ARG:NH2	2.46	0.48
1:A:1350:U:O2'	1:A:1796:A:N3	2.42	0.48
5:F:142:LEU:HD13	5:F:145:VAL:HG21	1.95	0.48
5:F:169:ARG:NH1	5:F:175:ASP:OD1	2.44	0.48
28:6:41:ARG:HD3	28:6:44:VAL:HG23	1.95	0.48
1:A:16:C:H5''	26:4:14:ASP:HB2	1.95	0.48
1:A:2154:U:C2	1:A:2158:A:N6	2.81	0.48
1:A:1303:U:H2'	1:A:1304:G:C8	2.49	0.48
1:A:1303:U:H2'	1:A:1304:G:H8	1.78	0.48
1:A:1656:G:HO2'	10:M:6:SER:HG	1.61	0.48
1:A:1781:A:H2'	1:A:1782:C:H6	1.78	0.48
1:A:2012:C:H2'	1:A:2013:U:C6	2.48	0.48
1:A:2278:U:OP1	1:A:2367:U:O2'	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2685:U:H2'	1:A:2686:C:C6	2.48	0.48
16:S:49:ASP:HA	16:S:52:GLN:HB2	1.95	0.48
1:A:2278:U:H2'	1:A:2279:G:H8	1.78	0.48
1:A:2471:G:OP1	12:O:45:ARG:NH1	2.37	0.48
1:A:938:C:H2'	1:A:939:G:H8	1.78	0.48
13:P:99:LYS:HB3	26:4:41:HIS:CE1	2.48	0.48
2:B:115:A:H2'	2:B:116:A:C8	2.49	0.48
3:D:145:GLU:HG2	3:D:151:GLY:C	2.39	0.48
9:L:4:TYR:CG	16:S:100:VAL:HG11	2.48	0.48
28:6:12:ARG:HE	28:6:44:VAL:HG12	1.77	0.48
18:U:73:THR:HB	18:U:106:LYS:HD2	1.96	0.48
30:8:16:ILE:HD13	30:8:25:VAL:HG22	1.95	0.48
1:A:293:A:H2'	1:A:294:A:C8	2.48	0.48
1:A:2122:A:H4'	1:A:2147:C:H4'	1.96	0.48
1:A:2771:U:H4'	4:E:44:ASP:OD1	2.14	0.48
1:A:150:U:H2'	1:A:151:C:C6	2.49	0.47
1:A:334:A:O2'	5:F:161:ARG:NH2	2.47	0.47
1:A:576:A:N1	1:A:799:G:O2'	2.40	0.47
1:A:1989:G:OP1	13:P:17:ARG:NH2	2.47	0.47
1:A:2404:C:OP1	29:7:24:LYS:NZ	2.47	0.47
21:X:162:LEU:HD22	21:X:173:LEU:HD13	1.95	0.47
1:A:121:G:H4'	1:A:149:A:H5'	1.95	0.47
1:A:269:C:H5''	1:A:271:U:H5'	1.96	0.47
1:A:580:A:H2'	1:A:581:U:C6	2.49	0.47
1:A:733:C:OP1	4:E:135:GLY:HA2	2.14	0.47
1:A:2098:U:O4	1:A:2131:G:O2'	2.32	0.47
1:A:2740:A:N7	36:A:3318:HOH:O	2.36	0.47
1:A:840:U:H2'	1:A:841:C:C6	2.48	0.47
1:A:1143:C:H4'	16:S:77:SER:HA	1.96	0.47
1:A:2052:C:H2'	1:A:2053:C:C6	2.49	0.47
32:J:19:ALA:HB1	32:J:69:PHE:HD2	1.79	0.47
32:J:100:ALA:HB2	32:J:106:PHE:HD2	1.79	0.47
1:A:719:G:C6	3:D:207:LYS:HB2	2.49	0.47
11:N:19:PRO:HA	11:N:27:LEU:HB3	1.97	0.47
27:5:25:THR:HG22	27:5:26:LYS:HE3	1.96	0.47
1:A:690:G:O2'	1:A:1622:A:N3	2.44	0.47
1:A:791:G:C8	5:F:49:SER:HB3	2.49	0.47
1:A:1980:U:H4'	4:E:133:THR:OG1	2.15	0.47
1:A:2341:A:H4'	22:Y:35:ASN:ND2	2.30	0.47
1:A:2602:U:C2	26:4:4:GLN:HA	2.49	0.47
2:B:39:U:H2'	2:B:40:U:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:X:63:VAL:HG13	21:X:74:THR:HG23	1.96	0.47
1:A:1276:C:H2'	1:A:1277:A:C8	2.50	0.47
1:A:1340:A:H2'	1:A:1341:A:C8	2.50	0.47
1:A:1757:G:N7	36:A:3313:HOH:O	2.35	0.47
1:A:2378:G:C6	1:A:2414:C:H1'	2.49	0.47
1:A:739:A:H4'	1:A:1258:G:N3	2.30	0.47
1:A:1424:C:H2'	1:A:1425:U:C6	2.50	0.47
1:A:1672:G:H2'	1:A:1673:C:C6	2.50	0.47
1:A:1840:A:H2'	1:A:1841:A:C8	2.49	0.47
1:A:2619:A:H2'	1:A:2620:G:C8	2.50	0.47
5:F:170:ASP:OD1	5:F:171:VAL:N	2.45	0.47
5:F:171:VAL:O	5:F:174:SER:OG	2.31	0.47
10:M:24:VAL:HG13	10:M:33:ALA:HB2	1.97	0.47
10:M:97:ARG:NH2	31:9:98:TYR:O	2.48	0.47
10:M:98:ILE:HD12	10:M:117:LEU:HB2	1.96	0.47
27:5:9:SER:HB3	27:5:45:TYR:CZ	2.49	0.47
1:A:1740:G:H5''	15:R:94:ARG:HD2	1.97	0.47
1:A:1892:C:H4'	1:A:1916:G:H8	1.79	0.47
1:A:2057:A:H2'	1:A:2058:A:C8	2.50	0.47
21:X:33:VAL:HG22	21:X:94:PHE:HB2	1.97	0.47
1:A:402:G:OP2	1:A:2393:U:O2'	2.32	0.47
1:A:837:C:H2'	1:A:838:A:H8	1.80	0.47
1:A:859:U:H2'	1:A:860:U:H5''	1.95	0.47
1:A:1045:G:H21	1:A:1075:A:H2	1.63	0.47
1:A:2051:C:H2'	1:A:2052:C:C6	2.50	0.47
1:A:2307:A:H8	1:A:2309:A:C5	2.33	0.47
1:A:2667:C:H5'	4:E:194:PRO:HA	1.97	0.47
6:G:8:TYR:OH	6:G:29:PRO:O	2.28	0.47
1:A:467:G:H4'	1:A:493:A:N1	2.29	0.47
1:A:979:G:OP2	25:2:11:SER:OG	2.23	0.47
1:A:2337:C:OP2	29:7:44:ARG:NH1	2.48	0.47
1:A:2454:C:O2	12:O:124:LYS:NZ	2.36	0.47
1:A:797:U:O2'	1:A:2047:A:N1	2.45	0.46
3:D:221:ARG:NH2	36:D:414:HOH:O	2.47	0.46
19:V:46:VAL:HG21	19:V:84:ILE:HD13	1.97	0.46
1:A:559:U:O2'	1:A:973:A:N1	2.48	0.46
1:A:1789:A:H2'	1:A:1790:A:C8	2.51	0.46
1:A:2220:U:H2'	1:A:2221:G:H8	1.80	0.46
1:A:2316:A:H2'	1:A:2317:G:C8	2.50	0.46
1:A:2636:C:H2'	1:A:2637:U:C6	2.51	0.46
3:D:29:PRO:HG2	3:D:34:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:115:TYR:OH	7:H:147:GLU:OE1	2.28	0.46
19:V:37:ALA:O	19:V:80:LYS:NZ	2.47	0.46
1:A:1708:U:H2'	1:A:1709:G:O4'	2.15	0.46
1:A:1184:G:H2'	1:A:1185:U:H6	1.81	0.46
1:A:1851:U:OP1	1:A:2397:G:O2'	2.25	0.46
1:A:2509:U:O2'	1:A:2634:U:OP1	2.25	0.46
13:P:56:LYS:HE2	13:P:87:TYR:O	2.15	0.46
1:A:38:A:N3	5:F:42:SER:HB3	2.30	0.46
1:A:647:U:H2'	1:A:648:C:C6	2.50	0.46
1:A:977:C:O2'	1:A:990:A:N3	2.43	0.46
1:A:1041:G:H1	1:A:1098:U:H3	1.61	0.46
1:A:1344:C:H2'	1:A:1345:G:O4'	2.15	0.46
1:A:2278:U:O2'	1:A:2361:C:O2	2.34	0.46
1:A:2636:C:H2'	1:A:2637:U:H6	1.81	0.46
18:U:97:VAL:HG12	18:U:99:ARG:HG2	1.98	0.46
22:Y:26:PHE:H	22:Y:29:GLN:HE21	1.64	0.46
1:A:13:A:O4'	1:A:517:A:N6	2.48	0.46
1:A:195:A:H61	1:A:198:C:H3'	1.81	0.46
1:A:1415:C:C5	1:A:1559:A:H5''	2.50	0.46
1:A:1425:U:H2'	1:A:1426:A:C8	2.50	0.46
1:A:207:A:H2'	1:A:208:C:O4'	2.16	0.46
3:D:135:ILE:O	3:D:167:ARG:NH2	2.49	0.46
32:J:27:VAL:HG21	32:J:76:PHE:HE1	1.81	0.46
1:A:571:C:H2'	1:A:572:A:H8	1.80	0.45
1:A:783:A:OP2	1:A:2058:A:O2'	2.32	0.45
1:A:1393:U:H2'	1:A:1394:C:H6	1.82	0.45
1:A:1784:C:O2'	3:D:258:THR:OG1	2.30	0.45
1:A:2142:U:H2'	1:A:2143:G:O4'	2.16	0.45
2:B:90:C:H5'	12:O:18:ARG:HG2	1.97	0.45
12:O:29:PHE:HB3	12:O:65:TRP:CE2	2.52	0.45
1:A:635:U:O2'	1:A:636:A:OP1	2.30	0.45
1:A:652:G:H5'	11:N:16:LYS:HB3	1.99	0.45
1:A:665:A:N3	1:A:2430:C:O2'	2.43	0.45
1:A:2025:G:H2'	1:A:2026:U:O4'	2.16	0.45
4:E:39:LYS:NZ	4:E:82:GLU:OE2	2.38	0.45
7:H:40:SER:HB2	7:H:61:THR:HG23	1.98	0.45
1:A:2626:A:H2'	1:A:2627:G:O4'	2.16	0.45
9:L:121:LYS:HE2	9:L:121:LYS:HB2	1.79	0.45
10:M:112:MET:HE1	31:9:33:VAL:HG11	1.98	0.45
1:A:454:G:N2	1:A:457:A:OP2	2.40	0.45
1:A:569:G:O2'	1:A:2006:A:OP1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:822:U:H2'	1:A:823:A:C8	2.51	0.45
1:A:929:G:OP1	29:7:64:ARG:NH2	2.50	0.45
1:A:2233:G:H2'	1:A:2234:A:C8	2.51	0.45
5:F:96:ASN:HB2	5:F:99:MET:HG3	1.98	0.45
1:A:774:G:H5'	1:A:775:G:OP1	2.16	0.45
1:A:1048:G:N1	1:A:1071:U:C2	2.84	0.45
1:A:1673:C:H2'	1:A:1674:A:C8	2.52	0.45
1:A:2298:A:N3	6:G:79:ILE:HD11	2.31	0.45
3:D:94:LEU:HD11	3:D:104:ILE:HD13	1.96	0.45
7:H:118:PRO:HD2	7:H:121:ILE:HD13	1.98	0.45
14:Q:28:CYS:HA	14:Q:92:ASP:HB3	1.99	0.45
19:V:86:LEU:HD11	19:V:92:LEU:HG	1.98	0.45
31:9:58:LYS:HA	31:9:58:LYS:HD2	1.75	0.45
1:A:835:A:O2'	1:A:836:U:O2	2.27	0.45
1:A:990:A:H2'	1:A:991:A:C8	2.52	0.45
26:4:37:HIS:ND1	26:4:38:LEU:O	2.49	0.45
1:A:2735:A:H5'	7:H:4:VAL:HG21	1.98	0.45
2:B:114:C:H2'	2:B:115:A:H8	1.81	0.45
12:O:43:THR:HG22	12:O:94:VAL:HG12	1.98	0.45
1:A:1069:C:H2'	1:A:1070:C:C6	2.52	0.45
1:A:1833:G:H2'	1:A:1834:A:O4'	2.17	0.45
10:M:38:ILE:HD11	10:M:111:PHE:HZ	1.82	0.45
30:8:1:MET:HE3	30:8:1:MET:HB2	1.86	0.45
1:A:58:G:O2'	1:A:73:A:N1	2.40	0.45
6:G:108:LEU:HD21	6:G:130:MET:HE1	1.98	0.45
1:A:388:U:H5''	23:Z:32:ASN:HB2	1.99	0.45
1:A:829:U:H2'	1:A:830:C:C6	2.52	0.45
1:A:2337:C:H5''	29:7:41:ARG:HD2	1.99	0.45
1:A:2439:C:H2'	1:A:2440:A:C8	2.52	0.45
2:B:29:A:H2'	2:B:30:C:C6	2.53	0.45
1:A:570:U:O3'	16:S:31:VAL:HG13	2.18	0.44
1:A:1796:A:H2'	1:A:1797:A:C8	2.53	0.44
1:A:2534:A:H4'	10:M:29:HIS:NE2	2.31	0.44
11:N:55:GLN:O	11:N:60:ARG:NH1	2.40	0.44
1:A:568:G:OP1	1:A:1242:U:O2'	2.30	0.44
1:A:617:A:N7	11:N:113:SER:HB2	2.31	0.44
1:A:982:C:OP1	16:S:47:TYR:OH	2.32	0.44
1:A:1843:U:H2'	1:A:1844:G:O4'	2.17	0.44
1:A:2154:U:N3	1:A:2158:A:N6	2.66	0.44
6:G:130:MET:HG3	6:G:154:ILE:HB	1.99	0.44
7:H:133:ILE:HG22	7:H:141:VAL:HG13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:41:VAL:HG11	17:T:103:ALA:HA	1.99	0.44
23:Z:53:ALA:HA	23:Z:56:MET:HE3	1.98	0.44
1:A:1425:U:H2'	1:A:1426:A:H8	1.83	0.44
6:G:126:GLY:O	6:G:158:THR:OG1	2.29	0.44
7:H:149:ARG:HA	7:H:162:VAL:HB	2.00	0.44
1:A:405:C:H2'	1:A:406:A:H8	1.82	0.44
1:A:1421:A:H2'	1:A:1422:G:O4'	2.17	0.44
1:A:1782:C:O2	3:D:254:LYS:NZ	2.46	0.44
33:K:133:ALA:HB1	33:K:138:LEU:HB2	1.99	0.44
1:A:938:C:H2'	1:A:939:G:C8	2.53	0.44
1:A:2272:C:OP2	27:5:2:ARG:NH1	2.50	0.44
36:A:4313:HOH:O	15:R:54:ARG:HD2	2.16	0.44
2:B:115:A:H2'	2:B:116:A:H8	1.81	0.44
11:N:51:GLU:OE2	29:7:56:ARG:NH1	2.51	0.44
1:A:86:U:H4'	1:A:104:U:H1'	1.99	0.44
1:A:376:C:H1'	36:A:3967:HOH:O	2.17	0.44
1:A:737:U:O2	1:A:2001:A:H1'	2.17	0.44
1:A:845:G:H2'	1:A:846:G:C8	2.52	0.44
1:A:1097:G:H2'	1:A:1098:U:C6	2.53	0.44
1:A:2269:G:H4'	1:A:2376:G:O2'	2.17	0.44
31:9:5:GLN:O	31:9:9:VAL:HG23	2.16	0.44
1:A:791:G:OP1	5:F:49:SER:HB2	2.18	0.44
1:A:1374:A:H5'	1:A:1456:A:H1'	1.99	0.44
1:A:1394:C:H2'	1:A:1395:U:H6	1.82	0.44
1:A:1627:A:H5'	1:A:1747:C:O2'	2.18	0.44
1:A:2346:C:H5''	29:7:50:ASN:ND2	2.33	0.44
1:A:2826:G:O2'	13:P:49:GLU:OE1	2.21	0.44
16:S:69:ALA:HB2	16:S:79:LEU:HD22	2.00	0.44
1:A:473:A:H1'	1:A:489:G:N2	2.32	0.44
1:A:2073:U:H2'	1:A:2074:U:C6	2.52	0.44
15:R:54:ARG:HB2	15:R:57:ASN:HB2	2.00	0.44
17:T:59:VAL:HG22	17:T:101:ILE:HG23	2.00	0.44
21:X:131:ILE:HG12	21:X:184:VAL:HA	1.98	0.44
1:A:654:G:N7	36:A:3341:HOH:O	2.36	0.44
1:A:803:U:H2'	1:A:804:C:H6	1.83	0.44
1:A:1081:G:H2'	1:A:1082:C:C6	2.53	0.44
1:A:1515:A:N6	1:A:1533:G:O2'	2.51	0.44
1:A:2006:A:H4'	16:S:34:VAL:HG21	1.99	0.44
1:A:2448:A:H2'	1:A:2449:C:C6	2.53	0.44
12:O:42:LEU:HG	12:O:97:ILE:HG13	2.00	0.44
17:T:24:LYS:HD3	17:T:92:TRP:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:G:OP1	28:6:33:ARG:NE	2.48	0.43
1:A:1253:G:O2'	1:A:1999:G:O6	2.24	0.43
1:A:1993:C:O2'	1:A:2810:A:N3	2.51	0.43
1:A:2079:U:H5''	8:I:24:GLY:HA3	1.99	0.43
1:A:2376:G:H5''	1:A:2377:U:O4'	2.18	0.43
1:A:2885:U:O2'	9:L:134:ALA:O	2.33	0.43
11:N:85:VAL:HB	11:N:94:THR:HG22	2.00	0.43
33:K:86:ILE:HD13	33:K:138:LEU:HD21	2.00	0.43
33:K:110:ALA:HB1	33:K:125:ALA:HB1	1.99	0.43
1:A:317:G:H2'	5:F:162:ASN:OD1	2.18	0.43
1:A:685:G:N7	36:A:3316:HOH:O	2.35	0.43
1:A:946:G:H2'	1:A:947:C:H2'	1.98	0.43
1:A:1911:C:H2'	1:A:1912:C:C6	2.53	0.43
1:A:1986:C:H5''	1:A:2710:C:O2'	2.18	0.43
1:A:2643:U:O2	1:A:2652:A:N7	2.50	0.43
1:A:570:U:H2'	1:A:571:C:H6	1.82	0.43
1:A:624:G:N7	11:N:74:ARG:NH1	2.65	0.43
1:A:840:U:H2'	1:A:841:C:H6	1.83	0.43
1:A:1381:U:H2'	1:A:1382:A:O4'	2.19	0.43
1:A:1914:A:H2'	1:A:1915:A:C8	2.53	0.43
1:A:2238:OMG:HM23	1:A:2238:OMG:H1'	1.70	0.43
13:P:17:ARG:HG2	13:P:21:PHE:CE2	2.52	0.43
13:P:35:LYS:HE3	13:P:100:CYS:SG	2.58	0.43
1:A:687:G:H2'	1:A:688:C:C6	2.53	0.43
1:A:1416:G:H2'	1:A:1417:G:H8	1.83	0.43
1:A:2137:U:H2'	1:A:2138:C:C6	2.53	0.43
4:E:17:THR:O	15:R:80:PRO:HG2	2.19	0.43
5:F:31:VAL:HG13	5:F:177:VAL:HG22	2.01	0.43
1:A:228:C:N4	1:A:2394:A:N3	2.64	0.43
1:A:622:A:H2'	1:A:623:A:C8	2.53	0.43
1:A:1811:G:O2'	3:D:253:THR:HG21	2.18	0.43
1:A:2187:C:H5''	23:Z:35:HIS:O	2.17	0.43
1:A:2456:A:H4'	12:O:56:ARG:HD2	1.99	0.43
4:E:26:THR:HG21	4:E:193:VAL:HB	2.00	0.43
31:9:17:LEU:HB2	31:9:51:LEU:HD23	1.99	0.43
1:A:1186:U:H2'	1:A:1187:C:H6	1.83	0.43
1:A:2499:C:H2'	1:A:2500:A:O4'	2.17	0.43
1:A:2760:U:OP1	4:E:169:ARG:NE	2.47	0.43
3:D:16:VAL:HG22	3:D:206:GLY:HA3	1.99	0.43
32:J:23:LEU:N	32:J:85:SER:O	2.46	0.43
1:A:83:G:H1	1:A:102:G:HO2'	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:U:H2'	1:A:491:G:O4'	2.18	0.43
1:A:2258:G:OP1	22:Y:18:SER:HB2	2.19	0.43
5:F:147:ILE:HD12	5:F:168:VAL:HG22	2.01	0.43
11:N:70:LYS:O	11:N:107:ARG:NH2	2.42	0.43
1:A:293:A:H8	1:A:293:A:OP2	2.01	0.43
1:A:719:G:C5	3:D:207:LYS:HB2	2.53	0.43
1:A:852:A:H2'	1:A:853:G:C8	2.54	0.43
1:A:1845:A:H2'	1:A:1846:U:O4'	2.18	0.43
1:A:2048:G:H2'	1:A:2488:C:O2'	2.19	0.43
1:A:2114:G:N1	1:A:2149:A:H1'	2.33	0.43
1:A:2442:G:H2'	1:A:2443:C:C6	2.54	0.43
2:B:22:U:H2'	2:B:23:G:C8	2.54	0.43
2:B:48:U:H2'	2:B:49:C:C6	2.54	0.43
12:O:65:TRP:HB2	12:O:105:GLU:HB2	2.01	0.43
1:A:314:A:H4'	1:A:316:A:N7	2.33	0.43
1:A:349:U:O2'	1:A:350:G:H8	2.02	0.43
1:A:579:U:H2'	1:A:580:A:C8	2.53	0.43
1:A:583:U:H2'	1:A:584:U:C6	2.53	0.43
1:A:2304:C:H2'	1:A:2305:G:O4'	2.19	0.43
24:1:3:ALA:HA	24:1:6:LEU:HD12	2.01	0.43
1:A:23:G:OP1	1:A:495:U:N3	2.40	0.43
1:A:669:C:H2'	1:A:670:G:H8	1.83	0.43
1:A:1017:A:C2	1:A:2475:G:H5'	2.54	0.43
1:A:2326:G:H2'	1:A:2327:C:C6	2.54	0.43
2:B:37:C:O2	14:Q:99:HIS:NE2	2.34	0.43
16:S:91:ASP:HB2	17:T:11:GLN:CD	2.43	0.43
1:A:586:A:H2'	1:A:587:G:C8	2.54	0.42
1:A:1037:G:N2	1:A:1100:G:O2'	2.52	0.42
1:A:1450:A:H2'	1:A:1451:A:C8	2.54	0.42
1:A:2114:G:H1	1:A:2149:A:H1'	1.84	0.42
1:A:2336:G:OP1	29:7:44:ARG:NH2	2.51	0.42
1:A:2362:G:N2	1:A:2365:A:OP2	2.41	0.42
4:E:9:LYS:NZ	4:E:195:GLY:O	2.41	0.42
12:O:17:ASN:O	12:O:39:ARG:HD3	2.18	0.42
17:T:2:TYR:CD1	17:T:13:LYS:HE2	2.54	0.42
21:X:100:ASP:OD1	21:X:101:HIS:N	2.51	0.42
1:A:245:G:O2'	1:A:375:A:N1	2.40	0.42
1:A:484:G:O2'	18:U:7:LEU:HA	2.18	0.42
1:A:710:U:H2'	1:A:711:G:H8	1.84	0.42
1:A:1144:C:OP1	16:S:92:ARG:NH2	2.48	0.42
1:A:1158:U:H2'	1:A:1159:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1532:C:H2'	1:A:1533:G:O4'	2.19	0.42
1:A:1856:G:N2	1:A:1859:A:OP2	2.33	0.42
1:A:1971:G:N7	36:A:3347:HOH:O	2.37	0.42
1:A:2038:U:H5'	1:A:2565:G:O4'	2.18	0.42
1:A:2334:C:H2'	1:A:2335:U:C6	2.55	0.42
33:K:81:LYS:O	33:K:85:GLY:N	2.51	0.42
1:A:3:U:H2'	1:A:4:C:C6	2.54	0.42
1:A:443:G:OP1	5:F:51:VAL:HG13	2.19	0.42
1:A:535:C:H2'	1:A:536:U:H5''	2.02	0.42
1:A:555:C:H2'	1:A:556:U:O4'	2.18	0.42
1:A:624:G:H2'	1:A:625:C:C6	2.54	0.42
1:A:1154:G:OP1	17:T:24:LYS:NZ	2.43	0.42
1:A:1722:C:H2'	1:A:1723:G:O4'	2.19	0.42
3:D:24:LEU:HD13	3:D:83:TYR:HB2	2.01	0.42
6:G:22:LEU:HD22	6:G:27:GLU:HB3	2.00	0.42
1:A:227:A:C2	1:A:2394:A:H1'	2.54	0.42
1:A:248:G:O5'	1:A:249:C:H5''	2.20	0.42
1:A:1393:U:H2'	1:A:1394:C:C6	2.54	0.42
1:A:2578:C:H2'	1:A:2579:G:H8	1.84	0.42
1:A:2624:U:H2'	1:A:2625:G:O4'	2.20	0.42
14:Q:35:HIS:ND1	14:Q:54:THR:OG1	2.47	0.42
1:A:1594:C:O2'	1:A:1600:A:N1	2.48	0.42
4:E:121:THR:HB	4:E:127:PHE:CD2	2.55	0.42
9:L:90:GLU:OE2	9:L:91:LYS:HG3	2.20	0.42
12:O:33:ALA:HB2	12:O:105:GLU:HG2	2.02	0.42
15:R:2:THR:HG22	15:R:7:GLN:HG3	2.01	0.42
21:X:138:CYS:HB3	21:X:171:VAL:HA	2.00	0.42
1:A:151:C:H2'	1:A:152:U:C6	2.54	0.42
1:A:272:A:H2'	1:A:273:A:C8	2.54	0.42
1:A:1256:A:H2'	1:A:1257:C:C6	2.55	0.42
1:A:1530:G:H2'	1:A:1531:A:C8	2.54	0.42
1:A:1657:G:O2'	1:A:1978:U:O4	2.32	0.42
1:A:1693:G:H2'	1:A:1694:U:C6	2.54	0.42
1:A:2232:U:H5''	36:A:4241:HOH:O	2.19	0.42
3:D:7:LYS:HA	3:D:8:PRO:HD3	1.91	0.42
5:F:1:MET:HG3	5:F:13:VAL:HG23	2.01	0.42
10:M:8:LEU:HD11	10:M:84:ALA:HB2	2.01	0.42
15:R:40:ARG:NH2	31:9:84:ASP:OD1	2.52	0.42
1:A:1357:C:H2'	1:A:1358:G:O4'	2.20	0.42
1:A:1460:U:H2'	1:A:1461:G:O4'	2.19	0.42
14:Q:91:PHE:HB2	14:Q:116:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:27:VAL:HG12	31:9:30:LYS:HD2	2.02	0.42
33:K:25:GLY:HA2	33:K:35:ILE:HD13	2.01	0.42
1:A:2095:U:H3	1:A:2168:G:H1	1.68	0.42
1:A:2544:G:H2'	1:A:2545:C:C6	2.55	0.42
1:A:2614:G:O2'	1:A:2768:A:N1	2.52	0.42
14:Q:26:ARG:HH21	14:Q:41:ILE:HD12	1.85	0.42
16:S:28:ARG:NH1	36:S:306:HOH:O	2.47	0.42
20:W:12:VAL:HG22	20:W:69:VAL:HG12	2.01	0.42
1:A:664:G:H1'	5:F:68:ARG:HE	1.84	0.42
1:A:1405:G:N2	1:A:1569:A:N7	2.68	0.42
1:A:1433:C:H2'	1:A:1434:U:C6	2.54	0.42
1:A:2175:U:H2'	1:A:2176:U:C6	2.55	0.42
1:A:2351:C:H2'	1:A:2352:G:O4'	2.19	0.42
3:D:164:LEU:HD12	3:D:164:LEU:HA	1.78	0.42
14:Q:93:ARG:HD2	14:Q:96:PHE:O	2.19	0.42
1:A:78:U:H2'	1:A:79:C:H6	1.83	0.41
1:A:584:U:H2'	1:A:585:C:C6	2.54	0.41
1:A:622:A:H5'	11:N:68:SER:HB2	2.01	0.41
1:A:699:U:H2'	1:A:700:U:O4'	2.19	0.41
1:A:731:U:H2'	1:A:732:C:C6	2.55	0.41
3:D:5:LYS:HB2	3:D:5:LYS:HE2	1.87	0.41
3:D:25:HIS:CG	3:D:80:ARG:HD2	2.54	0.41
4:E:23:ILE:HG23	4:E:190:LYS:HG3	2.02	0.41
9:L:105:VAL:HG11	9:L:122:LEU:HD22	2.01	0.41
15:R:8:GLN:O	15:R:12:GLU:HG3	2.20	0.41
1:A:364:U:H2'	1:A:365:A:H8	1.85	0.41
1:A:634:A:H2'	1:A:636:A:N7	2.35	0.41
1:A:732:C:H2'	1:A:733:C:C6	2.56	0.41
1:A:1078:A:H2'	1:A:1078:A:N3	2.35	0.41
1:A:1372:A:H1'	1:A:1373:C:C6	2.54	0.41
1:A:2107:G:H2'	1:A:2108:G:C8	2.54	0.41
4:E:84:ARG:HD2	4:E:84:ARG:HA	1.89	0.41
5:F:16:ARG:NH1	5:F:199:LEU:O	2.52	0.41
33:K:106:LEU:HD22	33:K:129:ILE:HG22	2.02	0.41
1:A:898:A:H2'	1:A:901:C:C5	2.55	0.41
2:B:40:U:H1'	2:B:45:A:H61	1.85	0.41
5:F:1:MET:HE3	5:F:19:GLY:HA3	2.02	0.41
10:M:104:ARG:CZ	15:R:33:VAL:HG11	2.50	0.41
18:U:18:ARG:HG3	18:U:76:VAL:HB	2.02	0.41
1:A:1912:C:H2'	1:A:1913:U:O4'	2.21	0.41
1:A:2009:U:O2'	1:A:2604:U:H5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2172:U:H2'	1:A:2173:G:C8	2.54	0.41
1:A:2501:U:H2'	1:A:2502:C:C6	2.56	0.41
2:B:93:C:H5''	21:X:24:ARG:CZ	2.49	0.41
6:G:104:LEU:HD23	6:G:108:LEU:HD12	2.01	0.41
9:L:13:ARG:HH22	9:L:49:ASP:HB3	1.84	0.41
18:U:3:VAL:HG21	18:U:58:ALA:HA	2.02	0.41
32:J:64:VAL:HG11	32:J:76:PHE:HZ	1.85	0.41
1:A:30:G:H2'	1:A:31:C:C6	2.56	0.41
1:A:150:U:H2'	1:A:151:C:H6	1.85	0.41
1:A:466:C:O2	1:A:470:A:N6	2.42	0.41
1:A:677:C:H2'	1:A:678:U:O4'	2.21	0.41
1:A:987:G:OP1	16:S:92:ARG:HB2	2.21	0.41
1:A:1770:A:H5'	1:A:2595:G:H4'	2.02	0.41
2:B:14:U:O3'	2:B:107:U:O2'	2.32	0.41
3:D:133:ARG:HB2	3:D:186:ALA:HB1	2.01	0.41
5:F:28:HIS:O	5:F:32:VAL:HG23	2.20	0.41
6:G:56:ASP:OD2	6:G:150:ARG:NH1	2.53	0.41
1:A:387:G:H1'	23:Z:29:PHE:HB3	2.01	0.41
1:A:1045:G:H1	1:A:1094:C:H42	1.68	0.41
1:A:1456:A:H2'	1:A:1457:A:H8	1.86	0.41
1:A:1773:A:H1'	1:A:1925:A:N6	2.35	0.41
6:G:147:ASP:OD1	6:G:147:ASP:N	2.53	0.41
11:N:78:ARG:HG3	11:N:111:MET:HE3	2.03	0.41
1:A:601:C:H2'	1:A:602:G:O4'	2.20	0.41
1:A:1048:G:C6	1:A:1049:G:C6	3.08	0.41
1:A:1114:G:O2'	30:8:37:GLN:HG2	2.21	0.41
1:A:1144:C:H5'	16:S:76:TYR:HE2	1.86	0.41
1:A:1174:G:H5''	17:T:83:HIS:NE2	2.35	0.41
1:A:1250:U:C4	1:A:1251:G:C6	3.09	0.41
1:A:1621:G:N1	1:A:1624:A:OP2	2.41	0.41
1:A:1795:A:H3'	1:A:1796:A:C8	2.56	0.41
1:A:2358:G:O2'	27:5:42:HIS:ND1	2.39	0.41
11:N:48:PRO:HB3	29:7:59:ARG:HG2	2.03	0.41
19:V:93:ASP:OD1	19:V:93:ASP:N	2.49	0.41
1:A:35:G:H1'	1:A:445:A:C4	2.56	0.41
1:A:151:C:H2'	1:A:152:U:H6	1.86	0.41
1:A:2318:G:O2'	1:A:2323:A:N1	2.53	0.41
4:E:30:VAL:O	4:E:185:ASN:HB3	2.21	0.41
14:Q:55:LEU:HA	14:Q:60:ARG:HD2	2.02	0.41
1:A:301:G:N1	1:A:304:A:OP2	2.46	0.41
1:A:578:U:H2'	1:A:579:U:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:851:G:H2'	1:A:852:A:O4'	2.21	0.41
1:A:949:A:H2'	1:A:950:A:C8	2.55	0.41
1:A:1296:G:H4'	28:6:7:PRO:HB2	2.02	0.41
1:A:1419:G:H2'	1:A:1420:A:H8	1.84	0.41
1:A:1635:G:H5''	1:A:1636:C:H5'	2.02	0.41
1:A:1673:C:H2'	1:A:1674:A:H8	1.86	0.41
1:A:2112:G:N2	1:A:2159:U:H5'	2.35	0.41
1:A:2228:A:H2'	1:A:2229:G:C8	2.56	0.41
1:A:2674:U:H2'	1:A:2675:G:O4'	2.20	0.41
1:A:2743:U:H4'	1:A:2744:A:OP1	2.19	0.41
5:F:163:LEU:HD12	5:F:163:LEU:HA	1.95	0.41
6:G:43:ALA:HB1	6:G:50:ILE:HD11	2.03	0.41
10:M:113:LYS:HD3	31:9:77:TRP:CE3	2.55	0.41
13:P:20:MET:HE2	13:P:20:MET:HB3	1.94	0.41
14:Q:52:ALA:HB3	14:Q:77:VAL:HB	2.02	0.41
21:X:22:LEU:HD22	21:X:28:LEU:HD12	2.03	0.41
23:Z:21:ALA:HB3	23:Z:23:ASN:HD21	1.85	0.41
27:5:21:LYS:HE3	27:5:21:LYS:HB3	1.93	0.41
31:9:95:ARG:HH21	31:9:101:GLU:CD	2.29	0.41
1:A:809:A:H5''	1:A:963:A:N1	2.36	0.41
1:A:847:G:N3	1:A:2255:A:H2'	2.36	0.41
1:A:1265:G:O2'	13:P:27:SER:HB3	2.20	0.41
1:A:1850:G:H4'	1:A:2398:A:H4'	2.02	0.41
1:A:2107:G:H2'	1:A:2108:G:H8	1.86	0.41
1:A:2366:G:H4'	14:Q:22:LEU:HD11	2.03	0.41
1:A:2665:A:H2'	1:A:2666:A:C8	2.55	0.41
2:B:58:A:H2'	2:B:59:A:O4'	2.21	0.41
9:L:114:LEU:HD12	9:L:114:LEU:HA	1.93	0.41
19:V:8:LYS:NZ	24:1:25:GLN:OE1	2.48	0.41
1:A:614:C:O2'	1:A:647:U:OP1	2.38	0.40
1:A:938:C:H1'	1:A:974:A:C8	2.56	0.40
1:A:1740:G:N7	36:A:3346:HOH:O	2.36	0.40
1:A:1998:U:H2'	1:A:1999:G:O4'	2.21	0.40
1:A:2360:A:H2'	1:A:2361:C:C6	2.56	0.40
3:D:107:PRO:HG2	3:D:110:VAL:HG21	2.02	0.40
3:D:205:LEU:HB3	3:D:210:ALA:HB3	2.02	0.40
4:E:121:THR:HG21	4:E:143:PRO:HB3	2.03	0.40
5:F:17:THR:HA	5:F:105:ARG:HG2	2.03	0.40
1:A:467:G:N1	1:A:470:A:OP2	2.43	0.40
1:A:471:A:H5''	20:W:41:ILE:HD12	2.03	0.40
1:A:1157:G:H2'	1:A:1158:U:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1424:C:H2'	1:A:1425:U:H6	1.85	0.40
1:A:1658:A:O2'	1:A:1664:G:N7	2.41	0.40
1:A:1933:U:H2'	1:A:1934:C:C6	2.57	0.40
1:A:2378:G:O6	1:A:2412:A:H8	2.05	0.40
5:F:167:ASP:HB2	5:F:182:TYR:OH	2.21	0.40
6:G:143:TYR:HE1	6:G:149:LEU:HD21	1.85	0.40
19:V:91:ASP:OD1	19:V:92:LEU:N	2.54	0.40
21:X:6:LEU:HG	21:X:53:LEU:HD22	2.03	0.40
1:A:2065:C:H2'	1:A:2066:U:C6	2.55	0.40
1:A:2806:G:H2'	1:A:2808:A:N7	2.37	0.40
17:T:5:ILE:HG12	17:T:14:VAL:HG21	2.02	0.40
1:A:317:G:H1'	1:A:1192:A:N1	2.36	0.40
1:A:1845:A:H61	1:A:1871:G:H1'	1.86	0.40
1:A:2128:G:H2'	1:A:2129:A:H8	1.87	0.40
1:A:2233:G:H2'	1:A:2234:A:H8	1.86	0.40
2:B:9:G:C2	2:B:10:A:C8	3.10	0.40
5:F:3:LEU:HD23	5:F:3:LEU:HA	1.92	0.40
8:I:79:LEU:HD23	8:I:79:LEU:H	1.87	0.40
1:A:152:U:H2'	1:A:153:U:C6	2.56	0.40
1:A:355:G:OP2	1:A:356:A:O2'	2.28	0.40
1:A:456:G:H2'	1:A:457:A:C8	2.56	0.40
1:A:906:A:H5''	1:A:2255:A:H61	1.87	0.40
1:A:1081:G:H2'	1:A:1082:C:H6	1.86	0.40
1:A:2472:G:O3'	12:O:126:PRO:HB3	2.22	0.40
1:A:2592:U:H2'	1:A:2593:C:C6	2.57	0.40
2:B:20:G:H2'	2:B:21:U:C6	2.56	0.40
23:Z:34:GLN:HB3	36:Z:101:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	270/273 (99%)	265 (98%)	5 (2%)	0	100	100
4	E	206/211 (98%)	200 (97%)	6 (3%)	0	100	100
5	F	198/200 (99%)	198 (100%)	0	0	100	100
6	G	177/179 (99%)	175 (99%)	2 (1%)	0	100	100
7	H	172/177 (97%)	171 (99%)	1 (1%)	0	100	100
8	I	107/148 (72%)	104 (97%)	3 (3%)	0	100	100
9	L	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
10	M	120/122 (98%)	120 (100%)	0	0	100	100
11	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
12	O	135/137 (98%)	134 (99%)	1 (1%)	0	100	100
13	P	117/129 (91%)	115 (98%)	2 (2%)	0	100	100
14	Q	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
15	R	112/116 (97%)	109 (97%)	3 (3%)	0	100	100
16	S	115/118 (98%)	115 (100%)	0	0	100	100
17	T	101/103 (98%)	101 (100%)	0	0	100	100
18	U	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
19	V	92/99 (93%)	91 (99%)	1 (1%)	0	100	100
20	W	89/104 (86%)	87 (98%)	2 (2%)	0	100	100
21	X	188/204 (92%)	187 (100%)	1 (0%)	0	100	100
22	Y	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
23	Z	75/78 (96%)	75 (100%)	0	0	100	100
24	1	59/63 (94%)	59 (100%)	0	0	100	100
25	2	54/58 (93%)	53 (98%)	1 (2%)	0	100	100
26	4	52/60 (87%)	52 (100%)	0	0	100	100
27	5	49/51 (96%)	49 (100%)	0	0	100	100
28	6	42/44 (96%)	42 (100%)	0	0	100	100
29	7	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
30	8	36/38 (95%)	36 (100%)	0	0	100	100
31	9	102/118 (86%)	100 (98%)	2 (2%)	0	100	100
32	J	109/166 (66%)	105 (96%)	4 (4%)	0	100	100
33	K	141/143 (99%)	136 (96%)	5 (4%)	0	100	100
All	All	3557/3800 (94%)	3506 (99%)	51 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	212/213 (100%)	211 (100%)	1 (0%)	81	90
4	E	160/162 (99%)	160 (100%)	0	100	100
5	F	157/158 (99%)	157 (100%)	0	100	100
6	G	153/153 (100%)	153 (100%)	0	100	100
7	H	137/141 (97%)	137 (100%)	0	100	100
8	I	85/107 (79%)	84 (99%)	1 (1%)	63	79
9	L	119/119 (100%)	118 (99%)	1 (1%)	73	86
10	M	102/102 (100%)	102 (100%)	0	100	100
11	N	106/106 (100%)	105 (99%)	1 (1%)	70	84
12	O	110/110 (100%)	110 (100%)	0	100	100
13	P	98/104 (94%)	98 (100%)	0	100	100
14	Q	86/87 (99%)	86 (100%)	0	100	100
15	R	96/98 (98%)	96 (100%)	0	100	100
16	S	87/88 (99%)	86 (99%)	1 (1%)	65	81
17	T	86/86 (100%)	86 (100%)	0	100	100
18	U	87/87 (100%)	87 (100%)	0	100	100
19	V	79/82 (96%)	79 (100%)	0	100	100
20	W	81/88 (92%)	81 (100%)	0	100	100
21	X	154/164 (94%)	153 (99%)	1 (1%)	78	89
22	Y	57/61 (93%)	57 (100%)	0	100	100
23	Z	66/67 (98%)	66 (100%)	0	100	100
24	1	54/55 (98%)	53 (98%)	1 (2%)	50	69
25	2	48/49 (98%)	48 (100%)	0	100	100
26	4	47/52 (90%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	5	47/47 (100%)	46 (98%)	1 (2%)	47	66
28	6	37/37 (100%)	35 (95%)	2 (5%)	20	29
29	7	54/55 (98%)	54 (100%)	0	100	100
30	8	34/34 (100%)	34 (100%)	0	100	100
31	9	90/101 (89%)	89 (99%)	1 (1%)	65	81
32	J	82/122 (67%)	82 (100%)	0	100	100
33	K	110/110 (100%)	110 (100%)	0	100	100
All	All	2921/3045 (96%)	2910 (100%)	11 (0%)	81	92

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	180	GLU
8	I	27	ARG
9	L	111	LYS
11	N	92	LEU
16	S	6	ARG
21	X	109	LEU
24	1	7	ARG
27	5	21	LYS
28	6	41	ARG
28	6	42	LEU
31	9	8	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	22	GLN
3	D	90	HIS
3	D	200	HIS
3	D	226	ASN
4	E	65	GLN
4	E	126	ASN
4	E	148	GLN
4	E	150	GLN
5	F	28	HIS
7	H	22	GLN
7	H	73	ASN

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Mol	Chain	Res	Type
7	H	111	HIS
10	M	91	GLN
11	N	104	HIS
11	N	106	GLN
13	P	9	HIS
13	P	89	ASN
15	R	53	ASN
16	S	44	GLN
17	T	69	HIS
17	T	102	GLN
18	U	23	GLN
19	V	61	ASN
19	V	87	GLN
20	W	48	ASN
21	X	161	HIS
22	Y	29	GLN
23	Z	23	ASN
23	Z	34	GLN
24	1	39	GLN
24	1	58	ASN
26	4	5	GLN
28	6	26	ASN
31	9	20	GLN
32	J	73	ASN
33	K	30	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2827/2892 (97%)	315 (11%)	6 (0%)
2	B	118/121 (97%)	14 (11%)	0
All	All	2945/3013 (97%)	329 (11%)	6 (0%)

All (329) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	34	U
1	A	45	G
1	A	51	G
1	A	63	A

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Mol	Chain	Res	Type
1	A	71	A
1	A	74	A
1	A	75	G
1	A	85	G
1	A	97	A
1	A	118	A
1	A	119	A
1	A	120	U
1	A	131	A
1	A	142	C
1	A	163	C
1	A	165	A
1	A	166	U
1	A	181	A
1	A	196	A
1	A	199	A
1	A	205	G
1	A	216	A
1	A	220	G
1	A	221	A
1	A	222	A
1	A	242	G
1	A	248	G
1	A	265	A
1	A	270	U
1	A	271	U
1	A	293	A
1	A	294	A
1	A	305	A
1	A	315	U
1	A	318	U
1	A	323	G
1	A	324	A
1	A	337	C
1	A	350	G
1	A	356	A
1	A	359	U
1	A	376	C
1	A	377	G
1	A	387	G
1	A	402	G
1	A	407	U

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Mol	Chain	Res	Type
1	A	434	A
1	A	445	A
1	A	447	C
1	A	472	G
1	A	481	A
1	A	482	G
1	A	485	G
1	A	495	U
1	A	496	A
1	A	499	A
1	A	520	A
1	A	521	G
1	A	522	C
1	A	523	A
1	A	536	U
1	A	537	U
1	A	538	G
1	A	553	A
1	A	563	U
1	A	565	A
1	A	593	A
1	A	603	U
1	A	604	A
1	A	622	A
1	A	627	A
1	A	635	U
1	A	636	A
1	A	660	A
1	A	676	U
1	A	700	U
1	A	716	G
1	A	719	G
1	A	720	A
1	A	737	U
1	A	754	A
1	A	765	G
1	A	766	G
1	A	772	A
1	A	774	G
1	A	775	G
1	A	779	A
1	A	795	G

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Mol	Chain	Res	Type
1	A	802	C
1	A	813	C
1	A	817	U
1	A	818	U
1	A	836	U
1	A	848	G
1	A	855	A
1	A	860	U
1	A	899	A
1	A	904	C
1	A	921	C
1	A	922	G
1	A	936	C
1	A	951	C
1	A	964	A
1	A	973	A
1	A	979	G
1	A	986	A
1	A	1002	U
1	A	1003	U
1	A	1016	U
1	A	1023	U
1	A	1035	U
1	A	1037	G
1	A	1050	U
1	A	1060	A
1	A	1078	A
1	A	1080	A
1	A	1090	C
1	A	1101	A
1	A	1102	G
1	A	1120	U
1	A	1122	U
1	A	1123	A
1	A	1125	C
1	A	1126	G
1	A	1133	A
1	A	1148	G
1	A	1162	G
1	A	1193	G
1	A	1199	G
1	A	1223	G

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Mol	Chain	Res	Type
1	A	1240	A
1	A	1243	G
1	A	1258	G
1	A	1259	A
1	A	1287	A
1	A	1288	A
1	A	1308	A
1	A	1316	U
1	A	1339	U
1	A	1347	G
1	A	1352	A
1	A	1365	A
1	A	1366	U
1	A	1379	A
1	A	1381	U
1	A	1403	G
1	A	1404	C
1	A	1414	A
1	A	1415	C
1	A	1439	G
1	A	1447	U
1	A	1469	G
1	A	1495	A
1	A	1496	A
1	A	1511	G
1	A	1556	A
1	A	1559	A
1	A	1568	U
1	A	1572	C
1	A	1573	U
1	A	1598	A
1	A	1624	A
1	A	1636	C
1	A	1637	U
1	A	1638	U
1	A	1664	G
1	A	1712	G
1	A	1717	U
1	A	1732	G
1	A	1736	G
1	A	1743	G
1	A	1751	G

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Mol	Chain	Res	Type
1	A	1760	A
1	A	1769	U
1	A	1771	A
1	A	1773	A
1	A	1787	C
1	A	1788	A
1	A	1795	A
1	A	1803	C
1	A	1816	A
1	A	1835	A
1	A	1845	A
1	A	1871	G
1	A	1872	A
1	A	1893	G
1	A	1914	A
1	A	1916	G
1	A	1917	G
1	A	1918	U
1	A	1923	A
1	A	1925	A
1	A	1942	U
1	A	1950	U
1	A	1952	C
1	A	1954	C
1	A	1957	A
1	A	1958	U
1	A	1959	G
1	A	1978	U
1	A	1979	G
1	A	1980	U
1	A	2008	A
1	A	2010	C
1	A	2017	6MZ
1	A	2018	A
1	A	2020	A
1	A	2030	U
1	A	2042	C
1	A	2043	G
1	A	2047	A
1	A	2048	G
1	A	2049	A
1	A	2056	7MG

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Mol	Chain	Res	Type
1	A	2080	G
1	A	2086	U
1	A	2098	U
1	A	2105	U
1	A	2107	G
1	A	2113	A
1	A	2114	G
1	A	2120	G
1	A	2144	G
1	A	2146	G
1	A	2149	A
1	A	2159	U
1	A	2160	A
1	A	2178	A
1	A	2185	A
1	A	2191	G
1	A	2198	A
1	A	2201	C
1	A	2212	A
1	A	2225	G
1	A	2226	G
1	A	2266	G
1	A	2270	U
1	A	2274	A
1	A	2292	U
1	A	2295	G
1	A	2298	A
1	A	2306	C
1	A	2308	G
1	A	2309	A
1	A	2312	A
1	A	2323	A
1	A	2332	G
1	A	2337	C
1	A	2341	A
1	A	2348	C
1	A	2358	G
1	A	2359	U
1	A	2370	G
1	A	2371	U
1	A	2372	C
1	A	2379	A

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Mol	Chain	Res	Type
1	A	2393	U
1	A	2412	A
1	A	2416	G
1	A	2417	A
1	A	2422	A
1	A	2428	U
1	A	2432	2MG
1	A	2435	A
1	A	2460	U
1	A	2462	C
1	A	2481	G
1	A	2489	G
1	A	2492	G
1	A	2493	U
1	A	2505	A
1	A	2516	G
1	A	2517	A
1	A	2522	G
1	A	2534	A
1	A	2553	A
1	A	2554	G
1	A	2559	A
1	A	2569	G
1	A	2589	A
1	A	2596	U
1	A	2600	U
1	A	2602	U
1	A	2616	U
1	A	2633	C
1	A	2648	G
1	A	2676	U
1	A	2677	U
1	A	2701	G
1	A	2713	U
1	A	2720	A
1	A	2731	G
1	A	2735	A
1	A	2744	A
1	A	2750	G
1	A	2752	A
1	A	2765	A
1	A	2767	G

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Mol	Chain	Res	Type
1	A	2786	G
1	A	2787	A
1	A	2795	G
1	A	2805	C
1	A	2806	G
1	A	2807	A
1	A	2808	A
1	A	2822	A
1	A	2823	U
1	A	2836	U
1	A	2859	A
1	A	2860	A
1	A	2867	C
1	A	2871	U
1	A	2872	U
1	A	2873	G
2	B	9	G
2	B	13	A
2	B	19	C
2	B	24	G
2	B	41	C
2	B	53	A
2	B	56	G
2	B	73	A
2	B	89	U
2	B	90	C
2	B	105	G
2	B	109	A
2	B	116	A
2	B	117	G

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	221	A
1	A	635	U
1	A	774	G
1	A	1871	G
1	A	2516	G
1	A	2743	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MG	A	2432	1	23,26,27	0.57	0	33,38,41	0.50	0
1	5MU	A	1926	1	19,22,23	0.46	0	27,32,35	0.62	0
1	2MA	A	2490	34,1	22,25,26	1.70	5 (22%)	32,37,40	3.47	13 (40%)
1	5MC	A	1949	1	19,22,23	0.58	0	26,32,35	0.61	0
1	1MG	A	735	1	23,26,27	3.05	8 (34%)	33,39,42	1.85	8 (24%)
1	6MZ	A	2017	1	22,25,26	2.36	5 (22%)	29,36,39	2.32	12 (41%)
1	OMU	A	2539	1	19,22,23	2.97	7 (36%)	25,31,34	1.83	5 (20%)
1	OMG	A	2238	1	23,26,27	0.52	0	32,38,41	0.45	0
1	2MG	A	1822	1	23,26,27	0.49	0	33,38,41	0.49	0
1	6MZ	A	1608	1	22,25,26	2.40	4 (18%)	29,36,39	2.36	10 (34%)
1	OMC	A	2485	34,1	19,22,23	0.56	0	25,31,34	0.68	0
1	7MG	A	2056	1	23,26,27	1.12	1 (4%)	27,39,42	0.92	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	A	2432	1	-	2/9/27/28	0/3/3/3
1	5MU	A	1926	1	-	0/7/25/26	0/2/2/2
1	2MA	A	2490	34,1	-	1/7/25/26	0/3/3/3
1	5MC	A	1949	1	-	0/7/25/26	0/2/2/2
1	1MG	A	735	1	-	0/7/25/26	0/3/3/3
1	6MZ	A	2017	1	-	2/9/27/28	0/3/3/3
1	OMU	A	2539	1	-	0/9/27/28	0/2/2/2
1	OMG	A	2238	1	-	1/9/27/28	0/3/3/3
1	2MG	A	1822	1	-	2/9/27/28	0/3/3/3
1	6MZ	A	1608	1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	A	2485	34,1	-	0/9/27/28	0/2/2/2
1	7MG	A	2056	1	-	0/7/37/38	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1608	6MZ	C6-N6	9.41	1.45	1.34
1	A	735	1MG	C2-N3	9.25	1.48	1.33
1	A	2017	6MZ	C6-N6	9.04	1.44	1.34
1	A	2539	OMU	C2-N1	7.65	1.50	1.38
1	A	735	1MG	C4-N3	6.68	1.49	1.34
1	A	2539	OMU	C2-N3	6.44	1.49	1.38
1	A	735	1MG	C2-N2	5.93	1.44	1.34
1	A	2539	OMU	C6-C5	5.32	1.47	1.35
1	A	2490	2MA	C6-N6	5.29	1.47	1.34
1	A	2056	7MG	C5-N7	4.56	1.41	1.35
1	A	2017	6MZ	C5-C4	-3.32	1.33	1.39
1	A	1608	6MZ	C5-C4	-3.25	1.33	1.39
1	A	2539	OMU	C4-N3	3.12	1.44	1.38
1	A	735	1MG	C5-C6	3.10	1.53	1.45
1	A	2539	OMU	O4-C4	-3.08	1.18	1.24
1	A	2017	6MZ	C5-N7	-3.02	1.33	1.39
1	A	2490	2MA	C5-C4	-2.97	1.33	1.39
1	A	1608	6MZ	C5-N7	-2.96	1.33	1.39
1	A	2490	2MA	C5-N7	-2.91	1.33	1.39
1	A	735	1MG	O6-C6	-2.85	1.17	1.23
1	A	735	1MG	C2-N1	2.84	1.42	1.37
1	A	2539	OMU	O2-C2	-2.78	1.18	1.23
1	A	2539	OMU	C5-C4	2.74	1.49	1.43
1	A	2490	2MA	C6-N1	-2.69	1.31	1.35
1	A	2017	6MZ	C8-N9	-2.57	1.33	1.37
1	A	1608	6MZ	C8-N9	-2.57	1.33	1.37
1	A	2490	2MA	C8-N9	-2.50	1.33	1.37
1	A	735	1MG	C5-N7	-2.49	1.34	1.39
1	A	735	1MG	C6-N1	2.49	1.45	1.40
1	A	2017	6MZ	C4-N9	-2.05	1.33	1.37

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2490	2MA	C5-C4-N3	-8.74	117.97	127.18
1	A	2490	2MA	N6-C6-N1	-8.58	105.46	117.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2490	2MA	CM2-C2-N3	7.73	128.70	117.13
1	A	2017	6MZ	N1-C2-N3	-5.88	119.69	128.58
1	A	1608	6MZ	N1-C2-N3	-5.82	119.77	128.58
1	A	2539	OMU	C4-N3-C2	-5.70	119.54	126.61
1	A	2490	2MA	N3-C4-N9	5.56	134.04	126.99
1	A	2490	2MA	C4-N9-C1'	-5.30	114.25	126.63
1	A	2490	2MA	C1'-N9-C8	5.26	138.76	127.09
1	A	1608	6MZ	C5-C4-N3	-5.24	119.50	126.72
1	A	735	1MG	C5-C4-N3	-4.92	120.56	128.39
1	A	2017	6MZ	C5-C4-N3	-4.60	120.39	126.72
1	A	2017	6MZ	C9-N6-C6	-4.40	118.77	122.85
1	A	2490	2MA	C5-C6-N6	4.34	134.03	123.29
1	A	2017	6MZ	N9-C8-N7	-4.04	108.20	113.94
1	A	1608	6MZ	N9-C8-N7	-4.02	108.23	113.94
1	A	1608	6MZ	C4-C5-C6	3.91	120.03	116.78
1	A	2490	2MA	CM2-C2-N1	-3.89	111.30	117.13
1	A	2539	OMU	N3-C2-N1	3.82	119.87	114.89
1	A	735	1MG	C1'-N9-C4	-3.73	115.47	126.49
1	A	2539	OMU	C5-C4-N3	3.72	120.01	114.80
1	A	735	1MG	C2-N3-C4	3.61	120.09	111.98
1	A	1608	6MZ	C9-N6-C6	-3.59	119.52	122.85
1	A	1608	6MZ	C2-N3-C4	3.58	120.56	111.83
1	A	2490	2MA	N9-C8-N7	-3.54	108.92	113.94
1	A	735	1MG	C1'-N9-C8	3.39	136.37	126.73
1	A	2017	6MZ	C2-N3-C4	3.35	120.02	111.83
1	A	2490	2MA	N3-C2-N1	-3.27	120.00	125.77
1	A	1608	6MZ	N3-C4-N9	3.22	132.65	127.17
1	A	2017	6MZ	C4-C5-C6	3.20	119.44	116.78
1	A	735	1MG	N9-C8-N7	-2.96	107.92	113.40
1	A	2539	OMU	O4-C4-C5	-2.95	120.08	125.16
1	A	1608	6MZ	C5-N7-C8	2.85	107.93	103.45
1	A	2490	2MA	C5-N7-C8	2.85	107.93	103.45
1	A	735	1MG	N9-C4-N3	2.77	131.49	125.95
1	A	2017	6MZ	C5-N7-C8	2.75	107.77	103.45
1	A	735	1MG	C5-C6-N1	2.74	120.08	115.02
1	A	2017	6MZ	N3-C4-N9	2.56	131.51	127.17
1	A	2490	2MA	C6-C5-C4	2.53	120.64	117.18
1	A	2056	7MG	C4-C5-N7	2.35	108.15	105.38
1	A	2017	6MZ	C4-C5-N7	-2.23	108.04	110.58
1	A	2056	7MG	C5-C4-N9	2.21	109.17	106.33
1	A	2017	6MZ	C4-N9-C1'	-2.18	121.52	126.63
1	A	1608	6MZ	C4-C5-N7	-2.18	108.09	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2539	OMU	O2-C2-N1	-2.10	120.06	122.80
1	A	2017	6MZ	C5-C4-N9	2.10	108.10	105.81
1	A	2490	2MA	C4-C5-N7	-2.10	108.18	110.58
1	A	2017	6MZ	C4-N9-C8	2.05	107.89	105.74
1	A	1608	6MZ	C4-N9-C8	2.05	107.89	105.74
1	A	735	1MG	C8-N7-C5	2.04	107.89	104.26

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	2238	OMG	C1'-C2'-O2'-CM2
1	A	2432	2MG	C3'-C4'-C5'-O5'
1	A	2017	6MZ	O4'-C4'-C5'-O5'
1	A	2432	2MG	O4'-C4'-C5'-O5'
1	A	2017	6MZ	C3'-C4'-C5'-O5'
1	A	1822	2MG	O4'-C4'-C5'-O5'
1	A	1822	2MG	C3'-C4'-C5'-O5'
1	A	2490	2MA	C4'-C5'-O5'-P

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	2432	2MG	1	0
1	A	1926	5MU	1	0
1	A	2017	6MZ	1	0
1	A	2238	OMG	1	0
1	A	1822	2MG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 203 ligands modelled in this entry, 203 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

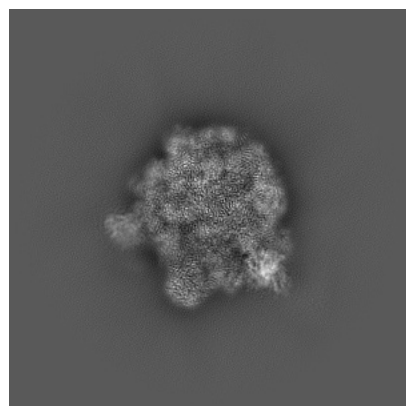
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72220. These allow visual inspection of the internal detail of the map and identification of artifacts.

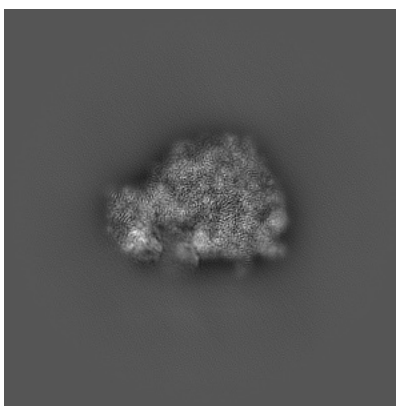
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

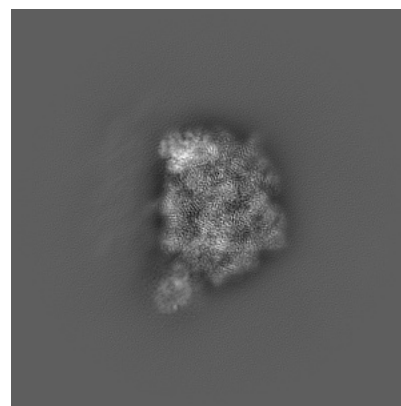
6.1.1 Primary map



X

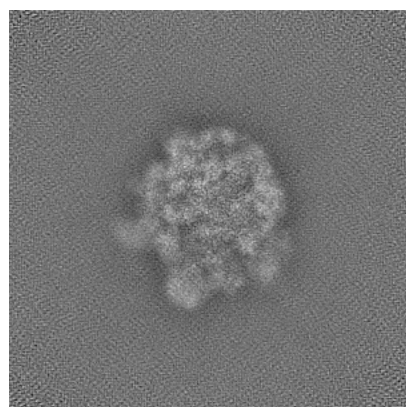


Y

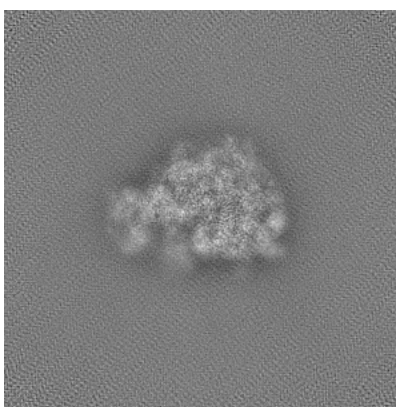


Z

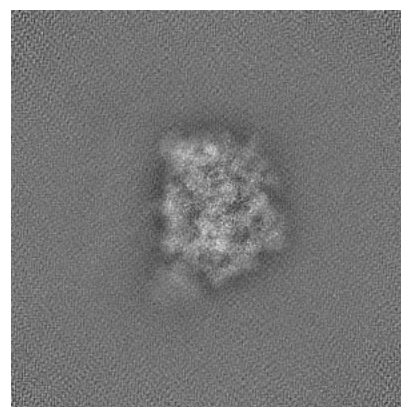
6.1.2 Raw map



X



Y

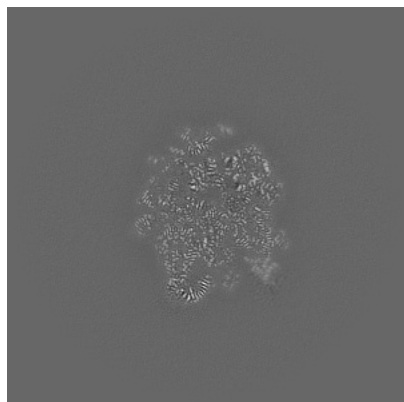


Z

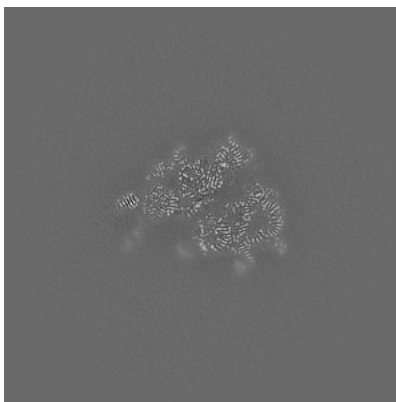
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

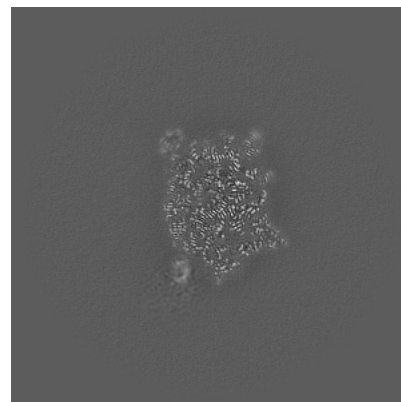
6.2.1 Primary map



X Index: 348

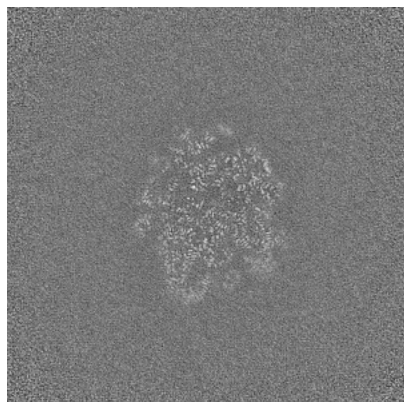


Y Index: 348

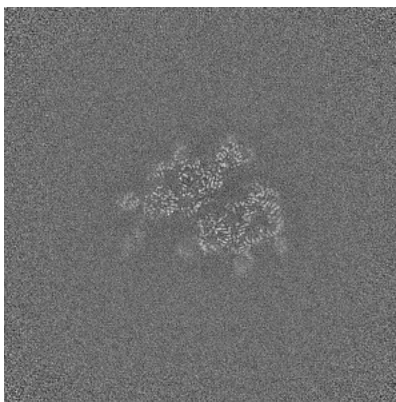


Z Index: 348

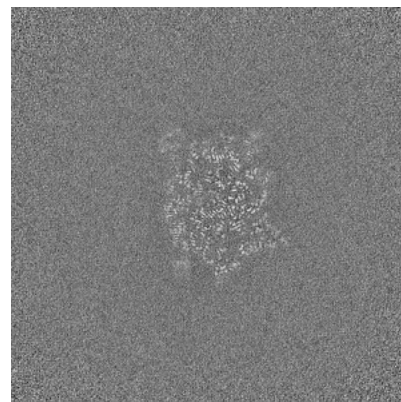
6.2.2 Raw map



X Index: 348



Y Index: 348

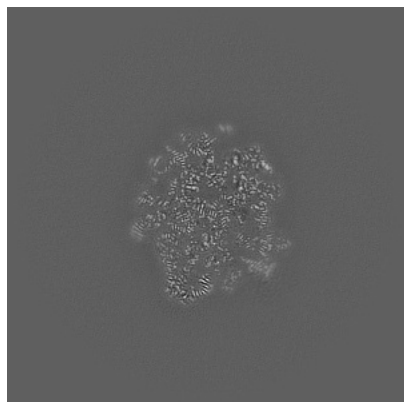


Z Index: 348

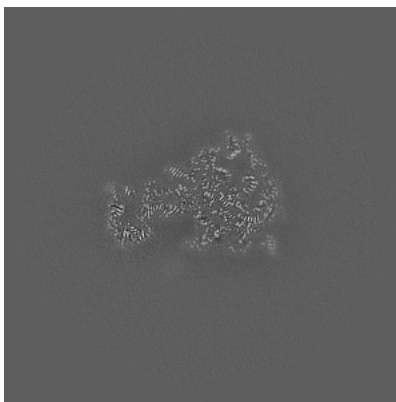
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

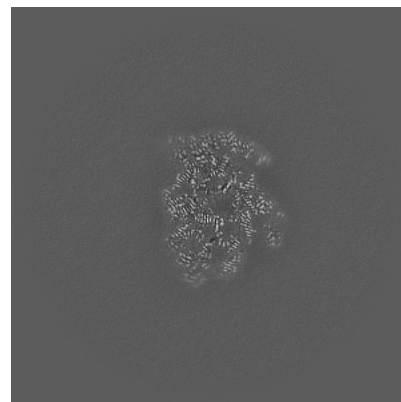
6.3.1 Primary map



X Index: 353

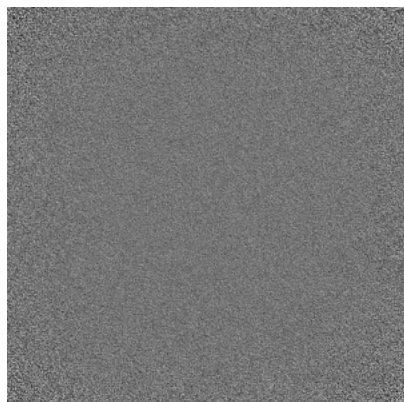


Y Index: 319

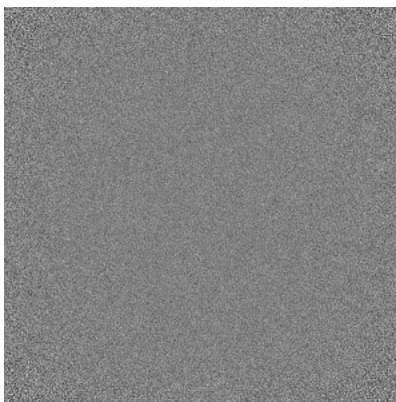


Z Index: 380

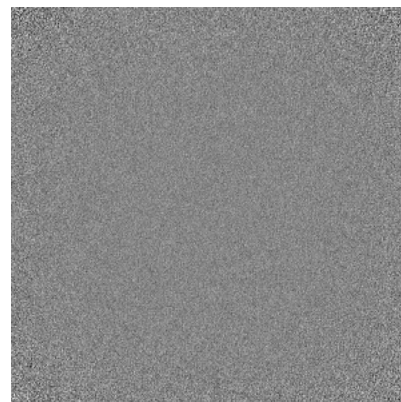
6.3.2 Raw map



X Index: 0



Y Index: 0

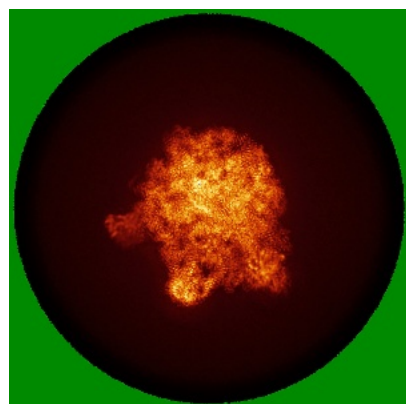


Z Index: 0

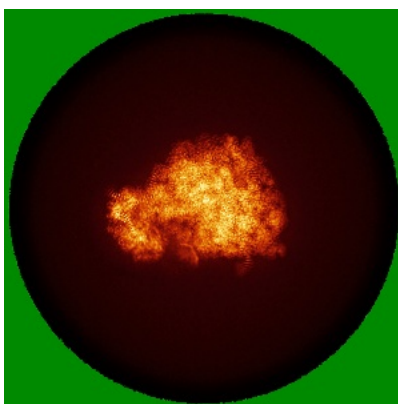
The images above show the largest variance slices of the map in three orthogonal directions.

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

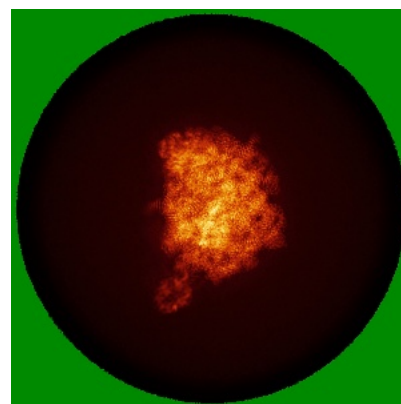
6.4.1 Primary map



X

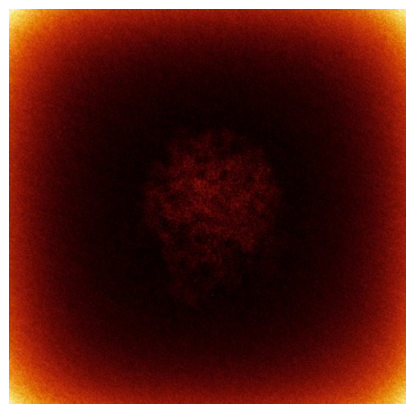


Y

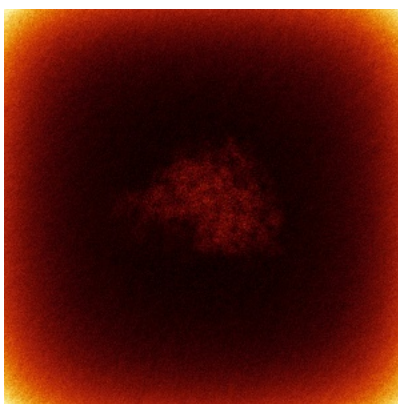


Z

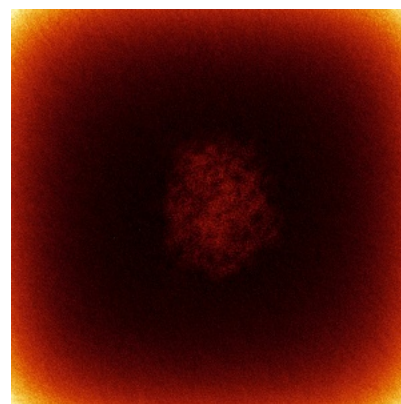
6.4.2 Raw map



X



Y

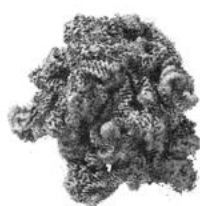


Z

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



X



Y



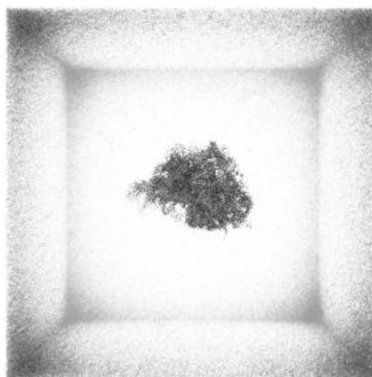
Z

The images above show the 3D surface view of the map at the recommended contour level 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

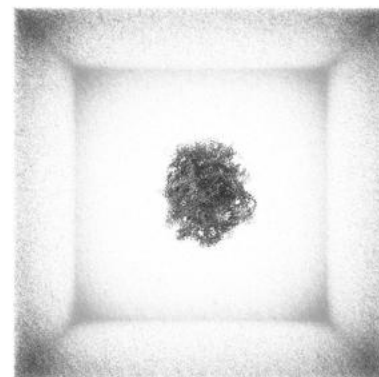
6.5.2 Raw map



X



Y



Z

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

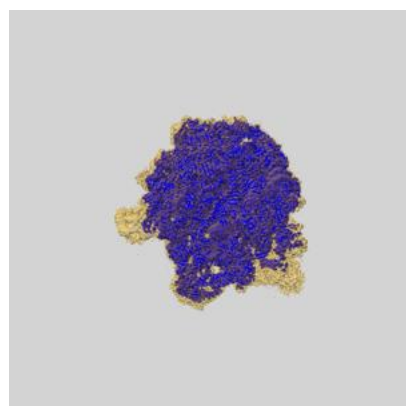
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

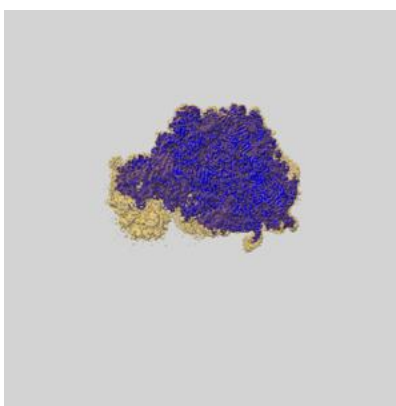
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

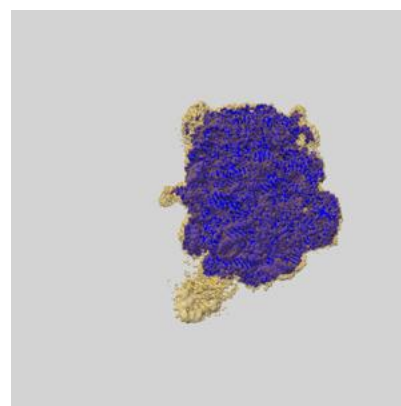
6.6.1 emd_72220_msk_1.map [i](#)



X



Y

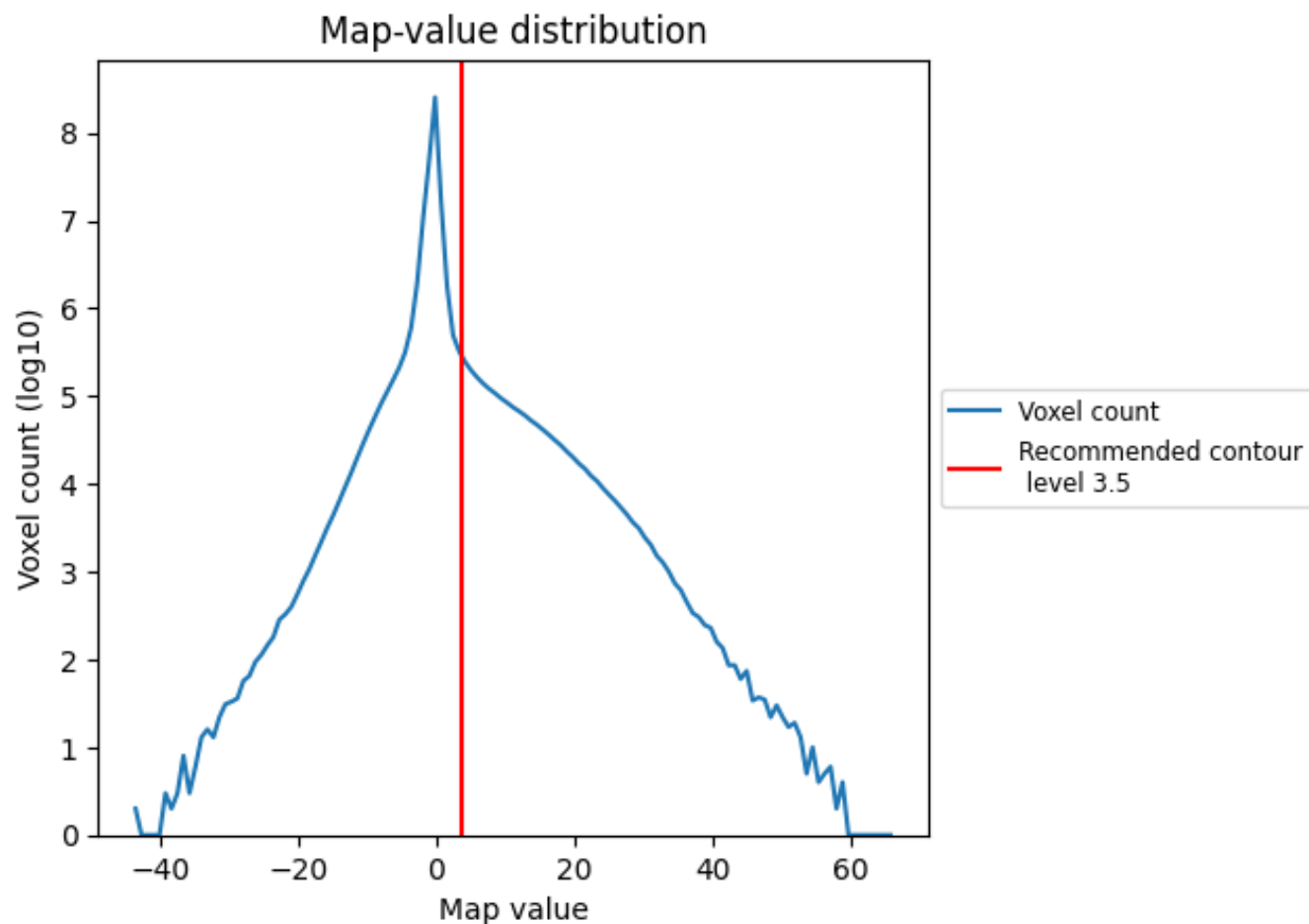


Z

7 Map analysis [i](#)

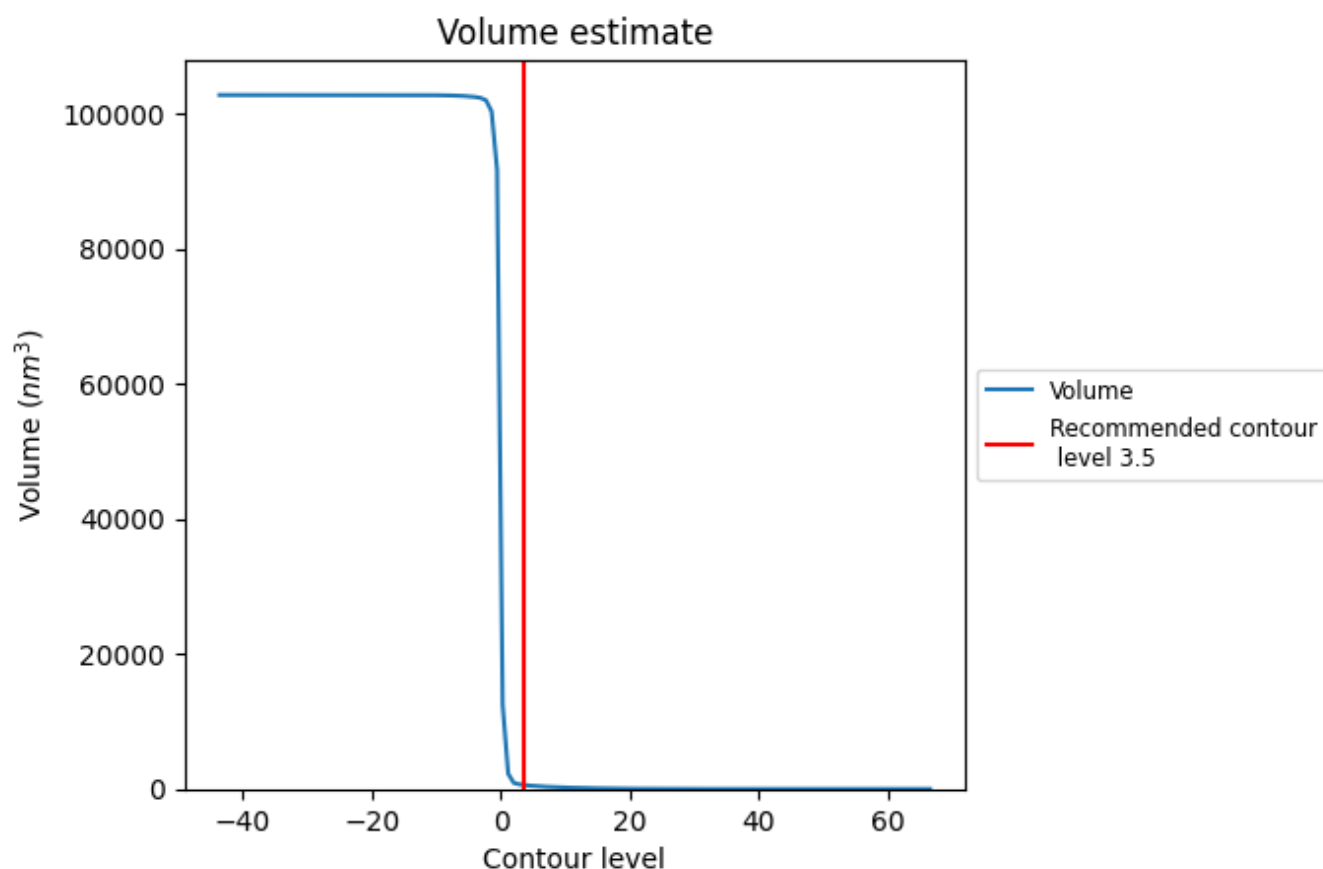
This section contains the results of statistical analysis of the map.

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.

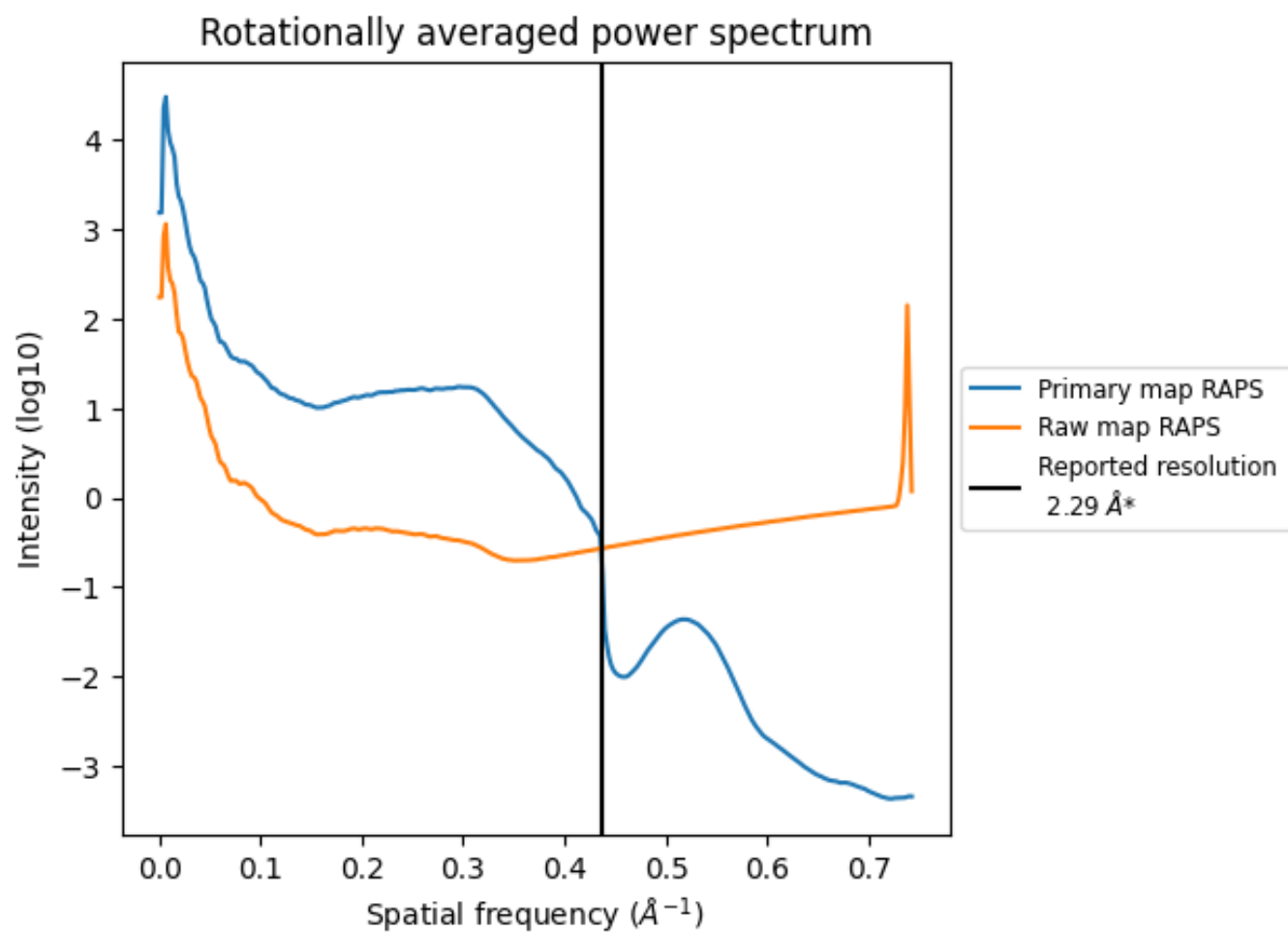
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 606 nm^3 ; this corresponds to an approximate mass of 548 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 ⓘ

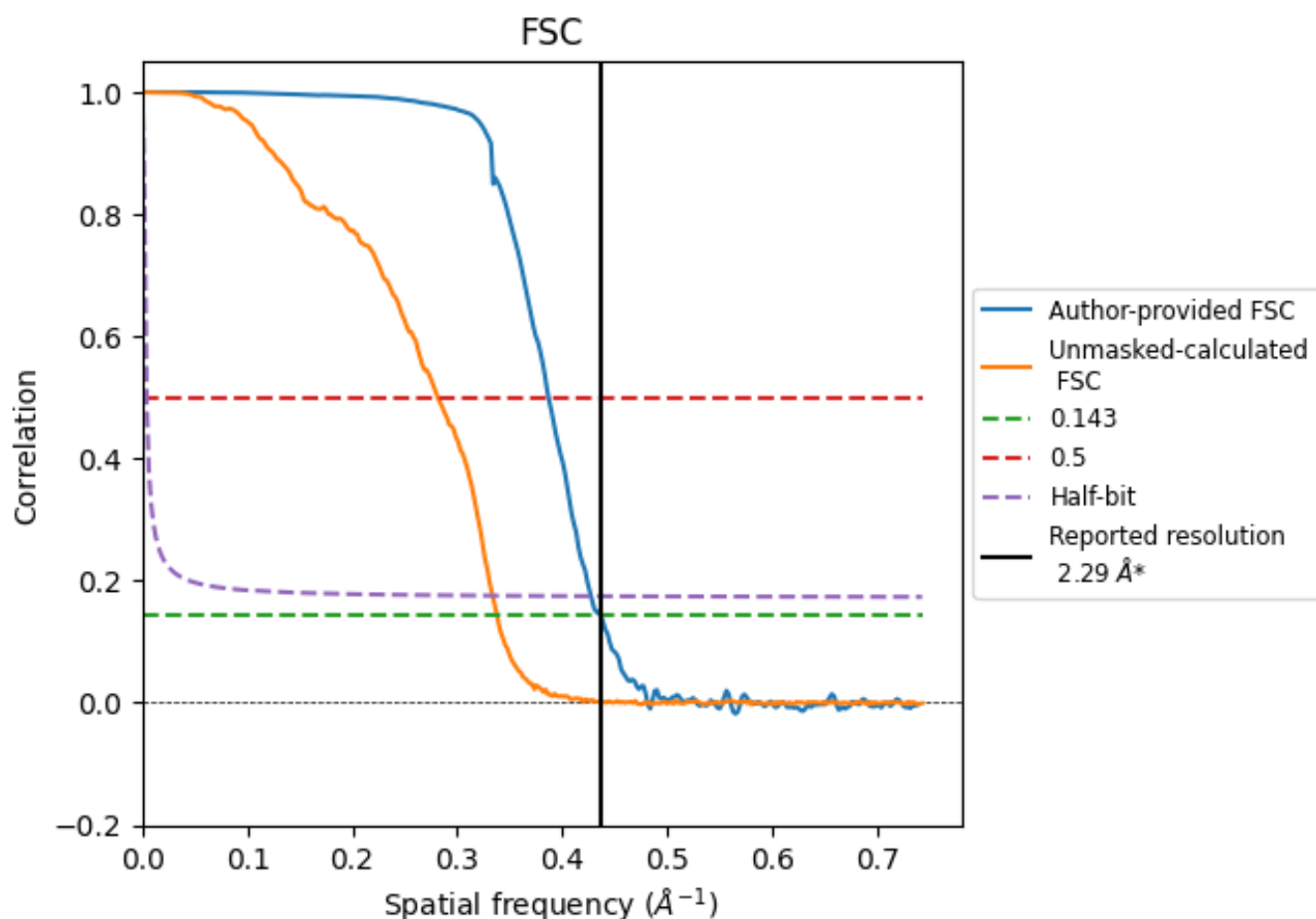


*Reported resolution corresponds to spatial frequency of 0.437 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.437 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

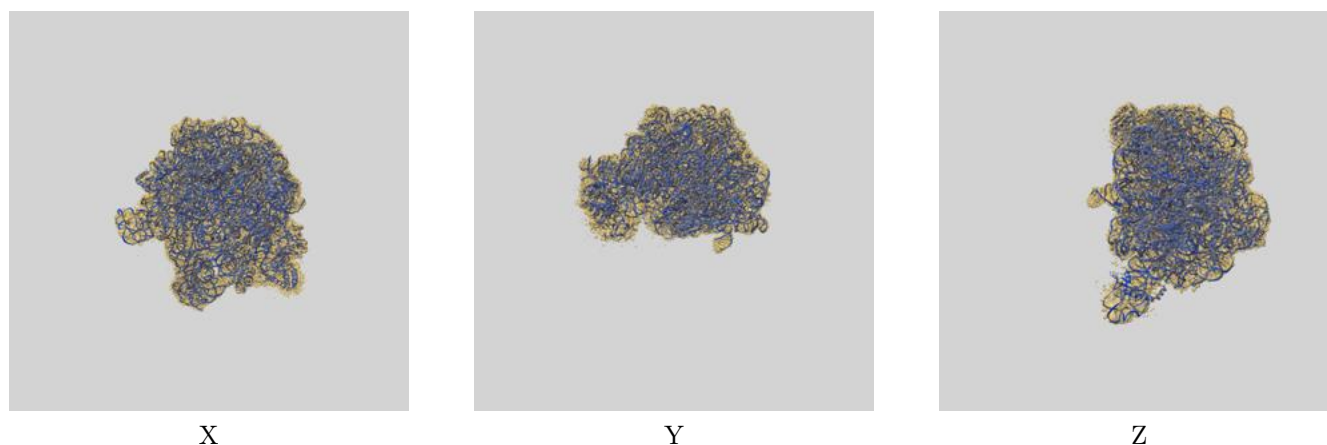
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.29	-	-
Author-provided FSC curve	2.29	2.58	2.34
Unmasked-calculated*	2.96	3.55	3.00

*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 2.96 differs from the reported value 2.29 by more than 10 %

9 Map-model fit [i](#)

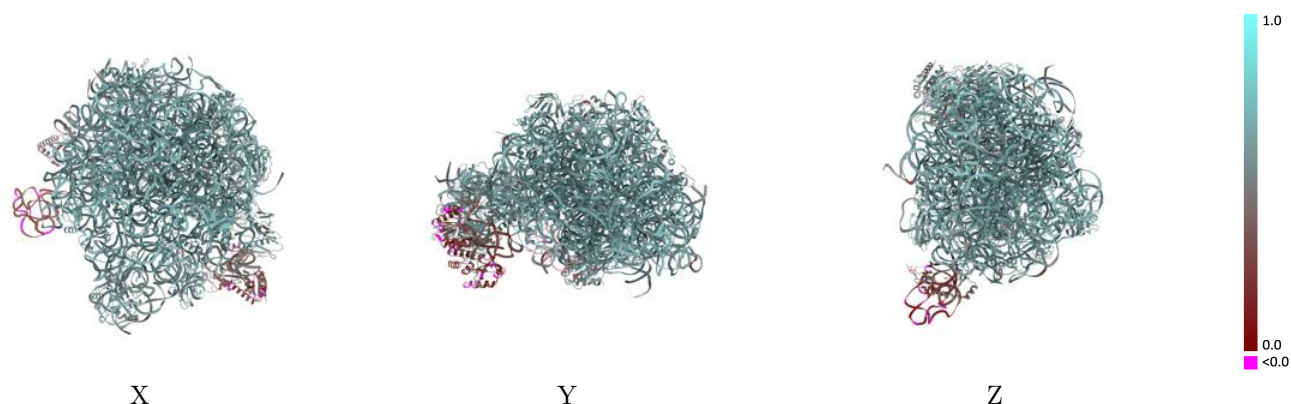
This section contains information regarding the fit between EMDB map EMD-72220 and PDB model 9Q44. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



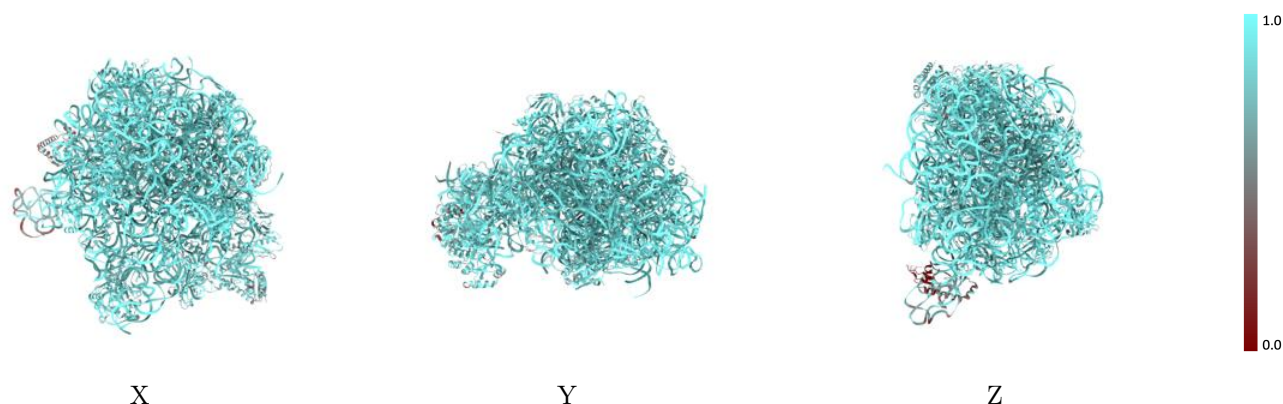
The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



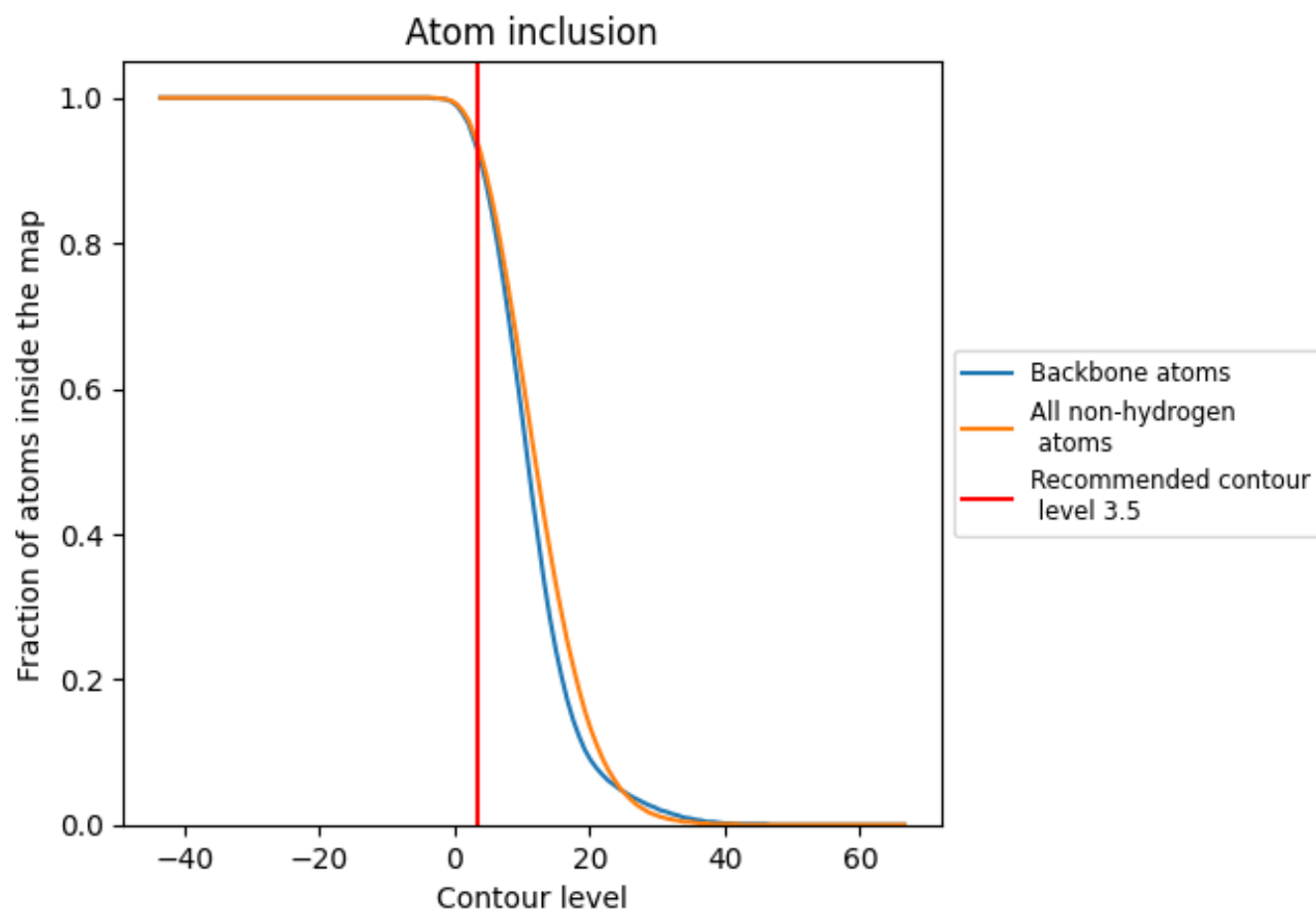
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 93% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9340	 0.6080
1	 0.8900	 0.6060
2	 0.9320	 0.6350
4	 0.9110	 0.6280
5	 0.8020	 0.5860
6	 0.9390	 0.6590
7	 0.9370	 0.6570
8	 0.9290	 0.6230
9	 0.7700	 0.4890
A	 0.9610	 0.6210
B	 0.9540	 0.6000
D	 0.9420	 0.6540
E	 0.9320	 0.6450
F	 0.9200	 0.6260
G	 0.8470	 0.5260
H	 0.8350	 0.5540
I	 0.4070	 0.4090
J	 0.7440	 0.2420
K	 0.8280	 0.2000
L	 0.9290	 0.6450
M	 0.8870	 0.6210
N	 0.9240	 0.6400
O	 0.8970	 0.6370
P	 0.9510	 0.6530
Q	 0.9000	 0.5930
R	 0.8700	 0.6190
S	 0.9530	 0.6540
T	 0.9220	 0.6220
U	 0.8880	 0.6340
V	 0.8800	 0.6060
W	 0.8760	 0.5790
X	 0.8490	 0.5760
Y	 0.9190	 0.6410
Z	 0.9040	 0.6400

