



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 03:10 AM UTC

PDB ID : 6YHS / pdb_00006yhs
EMDB ID : EMD-10809
Title : Acinetobacter baumannii ribosome-amikacin complex - 50S subunit
Authors : Nicholson, D.; Edwards, T.A.; O'Neill, A.J.; Ranson, N.A.
Deposited on : 2020-03-30
Resolution : 2.70 Å (reported)
Based on initial models : 5AFI, 5MDZ

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

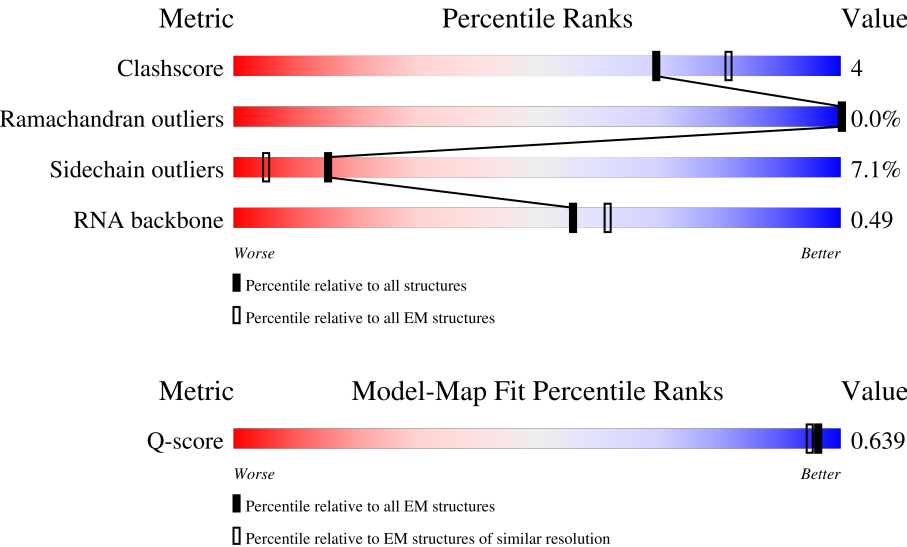
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 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	10327 (2.20 - 3.20)

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

Mol	Chain	Length	Quality of chain
1	1	2903	
2	5	117	
3	6	77	

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Mol	Chain	Length	Quality of chain
3	8	77	
4	A	274	
5	B	212	
6	C	200	
7	D	178	
8	E	177	
9	F	142	
10	G	122	
11	H	146	
12	I	137	
13	J	125	
14	K	116	
15	L	122	
16	M	119	
17	N	103	
18	O	110	
19	P	106	
20	Q	105	
21	R	98	
22	S	85	
23	T	78	
24	U	65	
25	V	58	
26	X	61	
27	Y	51	

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Mol	Chain	Length	Quality of chain
28	Z	44	91% 9%
29	a	64	91% ••••
30	b	38	84% 16%

2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 83514 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	2672	Total	C	N	O	P	0	0
			57324	25584	10504	18564	2672		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	115	Total	C	N	O	P	0	0
			2450	1095	440	800	115		

- Molecule 3 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	5	Total	C	N	O	P	0	0
			112	49	23	35	5		
3	8	8	Total	C	N	O	P	0	0
			169	76	32	53	8		

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	272	Total	C	N	O	S	0	0
			2109	1301	435	365	8		

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	211	Total	C	N	O	S	0	0
			1571	972	297	299	3		

- Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	199	Total	C	N	O	S	0	0
			1485	933	278	270	4		

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	176	Total	C	N	O	S	0	0
			865	513	176	176			

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	175	Total	C	N	O	S	0	0
			1327	838	238	250	1		

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	142	Total	C	N	O	S	0	0
			1122	717	200	201	4		

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	122	Total	C	N	O	S	0	0
			945	592	180	168	5		

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	144	Total	C	N	O	S	0	0
			1071	663	213	195			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	137	Total	C	N	O	S	0	0
			1086	687	210	184	5		

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	119	Total	C	N	O	S	1	0
			950	598	187	162	3		

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	115	Total	C	N	O	S	0	0
			864	532	175	156	1		

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	117	Total	C	N	O	S	0	0
			919	578	177	164			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	117	Total	C	N	O	S	0	0
			934	589	197	146	2		

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	103	Total	C	N	O	S	0	0
			806	506	155	142	3		

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	109	Total	C	N	O	S	0	0
			825	514	158	149	4		

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	92	Total	C	N	O	S	0	0
			717	457	129	130	1		

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	Q	102	Total	C	N	O		
			761	473	141	147	0	0

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	R	96	Total	C	N	O	S	
			753	472	142	138	1	0

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	S	76	Total	C	N	O	S	
			577	358	111	106	2	0

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	T	77	Total	C	N	O	S	
			631	395	130	104	2	0

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	U	61	Total	C	N	O	S	
			490	304	94	91	1	0

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	V	57	Total	C	N	O	S	
			453	281	87	81	4	0

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	X	54	Total	C	N	O	S	
			447	265	100	81	1	0

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	51	Total	C	N	O	S	0	0
			426	274	77	72	3		

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	44	Total	C	N	O	S	0	0
			362	222	85	53	2		

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	63	Total	C	N	O	S	0	0
			508	319	110	75	4		

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	38	Total	C	N	O	S	0	0
			294	179	64	47	4		

- Molecule 31 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
31	1	157	Total	Mg	0
			157	157	
31	5	3	Total	Mg	0
			3	3	

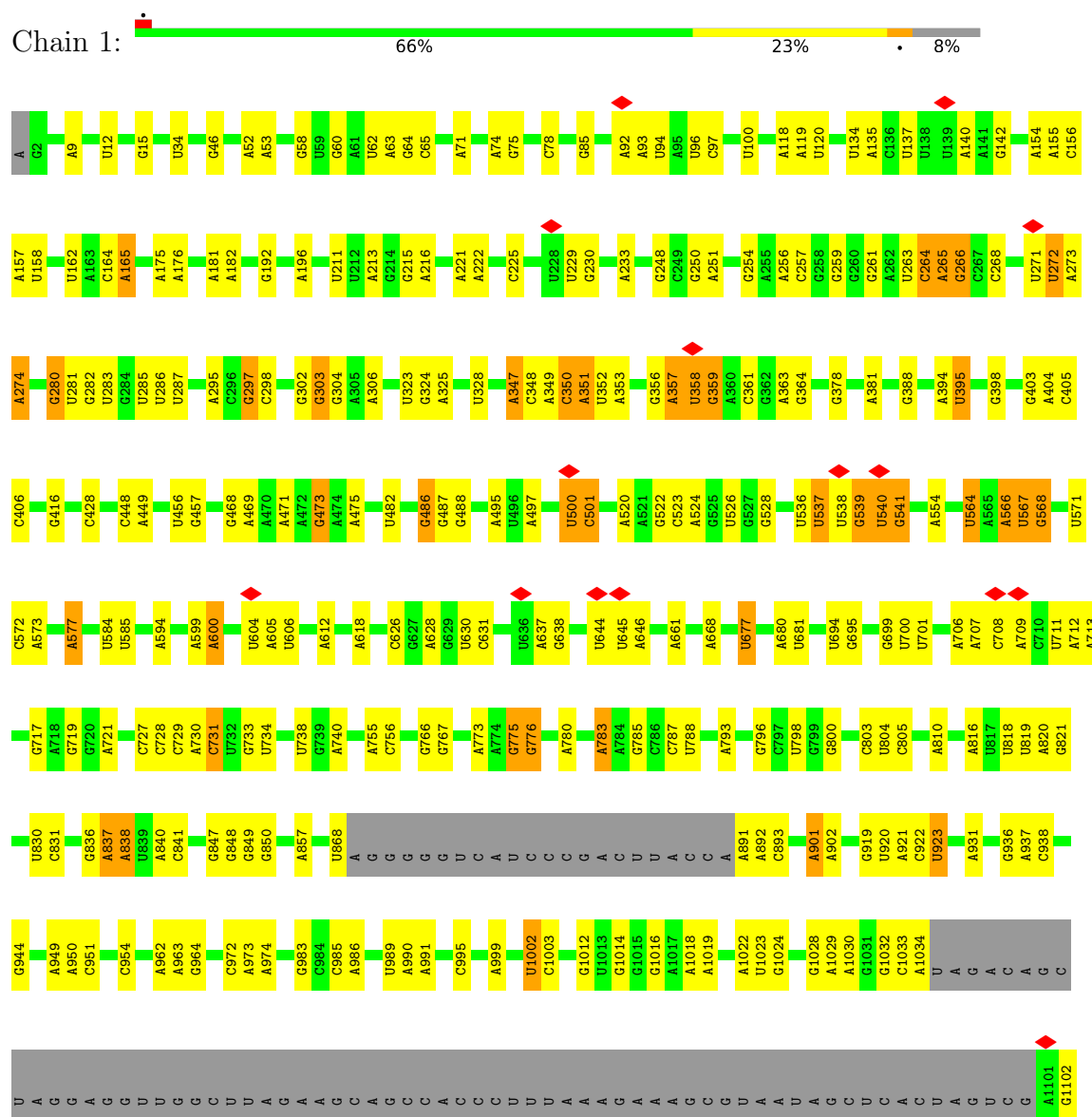
- Molecule 32 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
32	b	1	Total	Zn	0
			1	1	

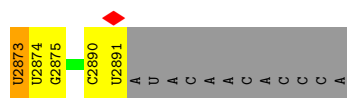
3 Residue-property plots

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

- Molecule 1: 23S ribosomal RNA



A2730	G2571	U2430	G2296	U	G	G2018	G1864	G1735	G1627	A	G1421	A1289	G1105
G2733	G2672	C2431	G2297	G	G	A2019	A1865	A1736	A1628	G	A1422	A1290	G1106
A2737	U2674	U2432	A2298	U	U	A2020	U1872	C1737	C1629	C	G1118	C1302	G1118
U2745	G2580	G2433	A2299	A	G	G2022	G1873	G1745	A1631	A	U1430	C1303	G1122
A2746	G2581	G2434	A2306	U	A	C2025	A1878	A1746	A1632	C	C1431	A1304	U1122
G2754	A2591	A2437	C2307	G	G	U2026	A1879	A1747	G1636	U	C1434	A1309	A1123
A2755	G2592	G2458	U2308	U	U	G2027	C1894	G1753	U1638	G	C1435	A1124	C1125
G2766	G2597	G2459	G2310	U	C	U2028	G1896	A1762	U1639	U	U1436	G1126	C1125
A2767	U2598	U2463	A2311	G	U	G2029		G1765	G1640	A	G1440	U1317	G1126
U2768	U2602	C2464	G2181	A	U	C2032			A1641	C		U1328	C1130
A2603	A2603	U2314	G2182	G	G		A1902	U1768	G1644	U	U1446	C1333	U1131
U2604	A2603	A2315	U2183	A	A	G2045	C1903		C1652	U	G1447	G1334	A1132
G2615	U2604	A2316	A2187	G	A	G2046	A1904	A1773	G1665	A	C1448	A1133	A1134
U2618	G2615	A2317	G2193	C	C	A2049	U1906	A1776	G1673	A	C1449	U1340	
U2624	G2615	G2318	U2194	U	U	G2050	A1907	C1777	U1674	G	G1455	A1341	A1161
G2635	U2618	G2470	G2200	G	G	A2051	A1908	U1778	A1681	A	A1456	A1342	C1162
C2638	U2624	U2480	A2201	A	A	C2052	U1912	U1779	G1686	C	A1457	A1343	U1163
U2786	G2635	G2487	A2202	C	C	G2054	C1913	A1780	G1698	A	A1458	G1349	U1164
A2787	G2638	A2491	A2212	U	U	U2057	A1916	U1785	G1701	U	G1463	C1350	U1165
U2789	U2639	A2492	G2213	C	C	U2058	A1917	C1786	U1702	U	U1464	A1353	G1166
G2647	G2647	U2493	A2214	U	U	A2059	U1918	U1787	U1703	U	U1470	U1367	U1167
C2792	G2650	G2501	U2232	U	U	G2061	G1919	C1789	G1704	A	U1471	A1168	U1169
C2793	A2651	U2507	U2233	C	C	C2062	A1926	A1791	U1705	C	U1472	A1170	A1170
U2794	G2652	U2508	U2234	U	U	U2064	U1927	A1792	G1706	A	U1473	C1171	G1172
A2797	G2658	G2509	G2235	G	G	U2075	U1928	U1797	U1706	U	U1474	G1388	G1175
U2798	A2659	U2518	A2236	U	U	G2076	U1929	A1799	U1706	U	U1476	A1371	G1175
G2800	G2660	G2518	G2240	G	G	U2086	U1944	G1800	U1709	U	U1477	A1374	G1194
U2807	G2674	C2522	C2250	A	A	U	U1952	C1805	G1710	U	C1481	U1375	G1226
G2809	U2678	A2523	A2257	C	C	G	G1953	G1806	A1711	U	A1482	G1376	A1235
A2810	A2679	A2531	A2257	C	C	A	C1956	U1807	U1712	U	A1483	A1380	G1236
A2824	C2692	A2536	A2262	U	U	C	A1959	A1818	G	G	U1485	A1383	U1237
U2834	C2693	U2537	A2263	C	C	U	U1960	G1835	A	A	C1486	U1396	G1238
G2835	C2697	U2543	G2268	U	U	C	G1961	A1836	C	C	G1489	G1397	A1241
G2837	G2703	U2544	U2272	U	U	U	U1980	A1837	U	U	G1490	U1398	G1244
G2838	U2715	C2545	A2276	A	A	G	U1982	A1847	C	C	U1491	G1399	G1252
U2850	U2718	G2555	A2277	C	C	U	C1986	U1848	U	U	A1492	U1400	A1253
A2856	G2719	G2556	U2280	A	A	U	A2010	U1853	C	C	C1494	A1401	G1254
G2720	G2720	C2562	G2281	C	C	A	U2011	G1857	U1726	U	U1495	A1402	U1255
G2721	G2721	C2563	A2287	C	C	G	C2012	G1858	G1727	U	C1496	U1403	A1256
A2722	A2722	U2564	A2287	C	C	U	G2013	U1859	A1728	U	C1497	G1404	A1256
C2869	A2729	A2566	U2294	C	C	A	C2014	A1860	G1729	U	U1497	A1405	G1259
A2872			C2295	C	C	A	U2015	G1862	C1734	U	U1499	A1406	G1260
							U2016	A1861			G1500	A1407	G1271
							U2017	G1863			A1504	U1408	A1274
											U1511	C1416	A1288
											U	G1417	



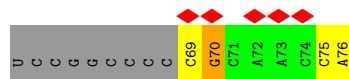
- Molecule 2: 5S ribosomal RNA



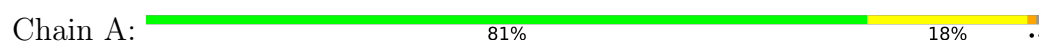
- Molecule 3: E-site tRNA



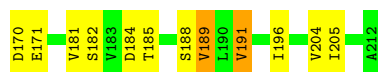
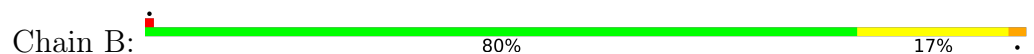
- Molecule 3: E-site tRNA



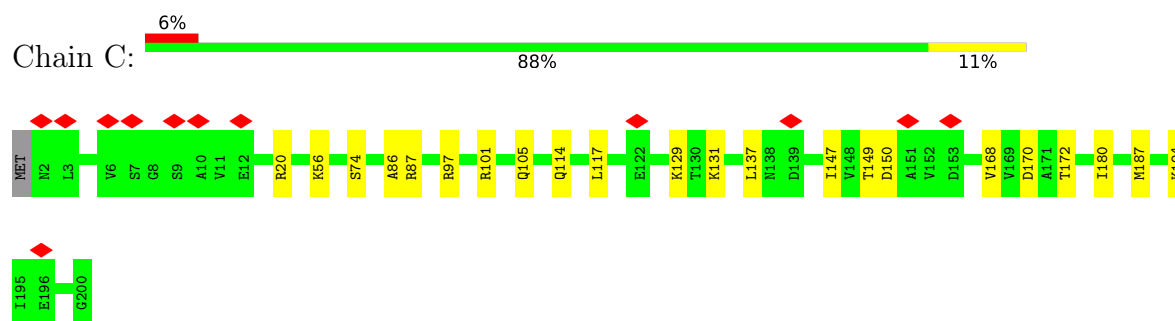
- Molecule 4: 50S ribosomal protein L2



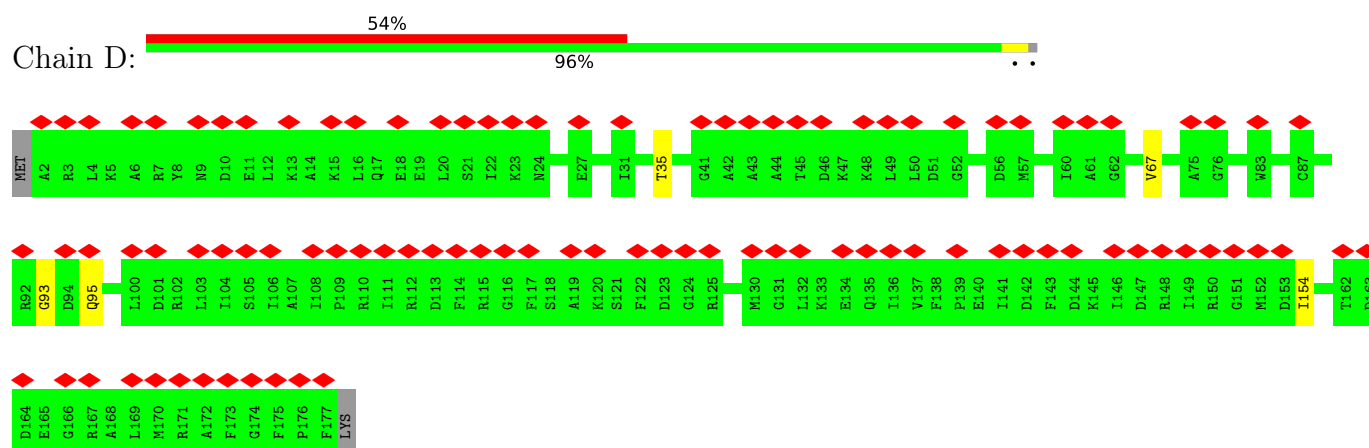
- Molecule 5: 50S ribosomal protein L3



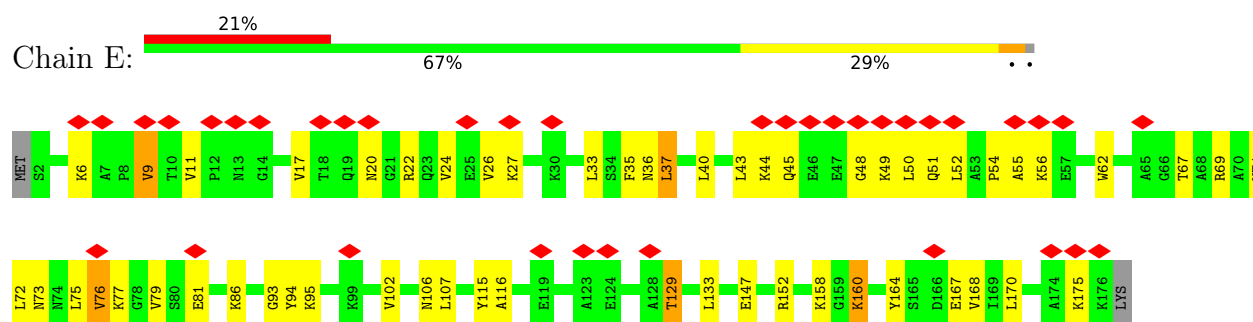
- Molecule 6: 50S ribosomal protein L4



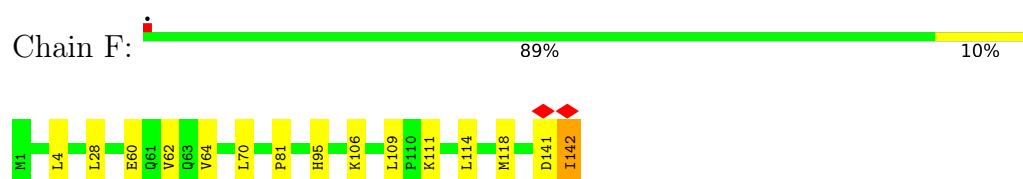
- Molecule 7: 50S ribosomal protein L5



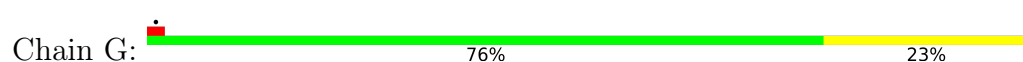
- Molecule 8: 50S ribosomal protein L6



- Molecule 9: 50S ribosomal protein L13

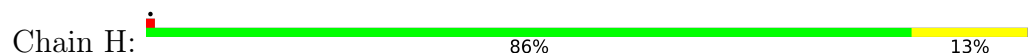


- Molecule 10: 50S ribosomal protein L14

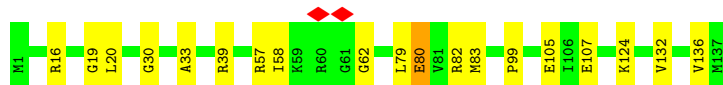
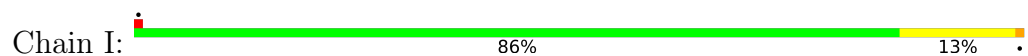




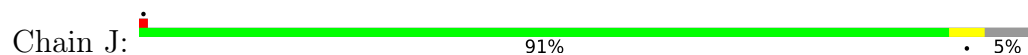
- Molecule 11: 50S ribosomal protein L15



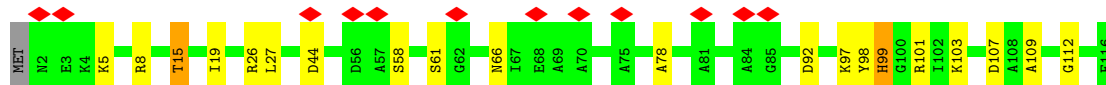
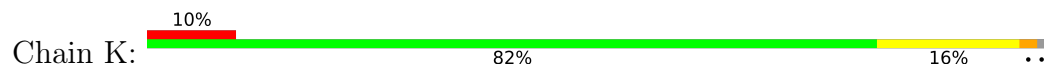
- Molecule 12: 50S ribosomal protein L16



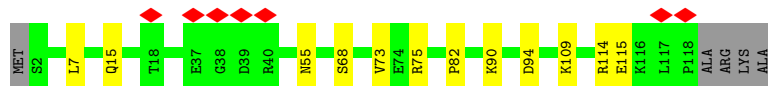
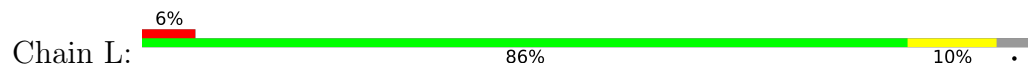
- Molecule 13: 50S ribosomal protein L17



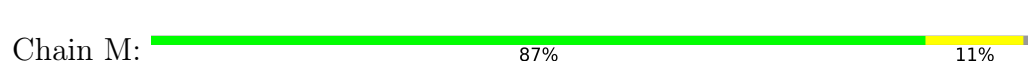
- Molecule 14: 50S ribosomal protein L18



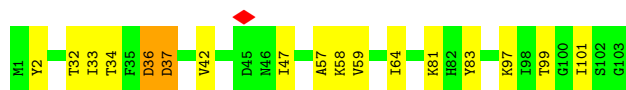
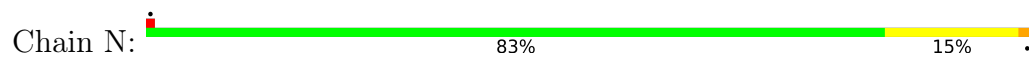
- Molecule 15: 50S ribosomal protein L19



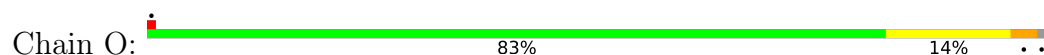
- Molecule 16: 50S ribosomal protein L20



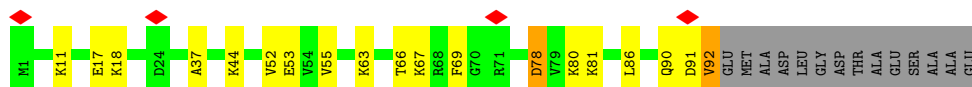
- Molecule 17: 50S ribosomal protein L21



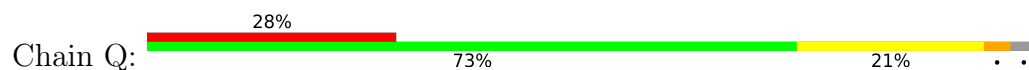
- Molecule 18: 50S ribosomal protein L22



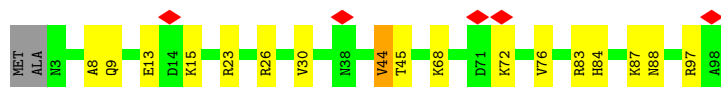
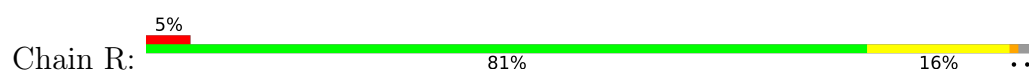
- Molecule 19: 50S ribosomal protein L23



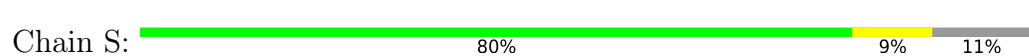
- Molecule 20: 50S ribosomal protein L24



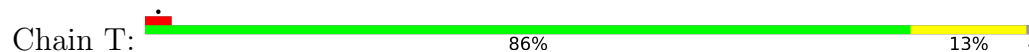
- Molecule 21: 50S ribosomal protein L25



- Molecule 22: 50S ribosomal protein L27

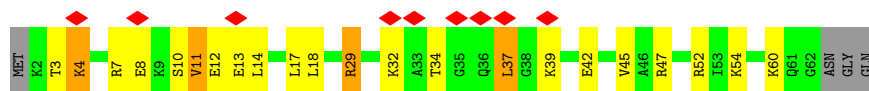


- Molecule 23: 50S ribosomal protein L28

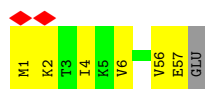
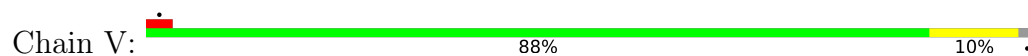




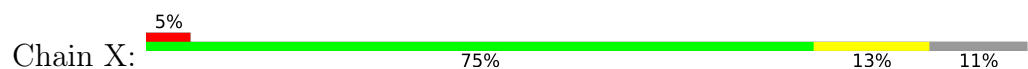
- Molecule 24: 50S ribosomal protein L29



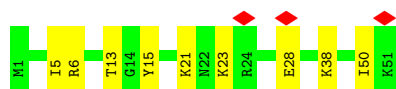
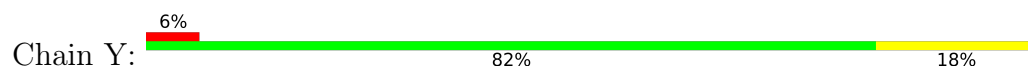
- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L32



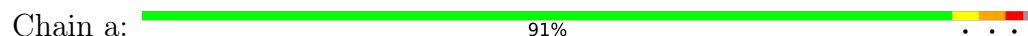
- Molecule 27: 50S ribosomal protein L33



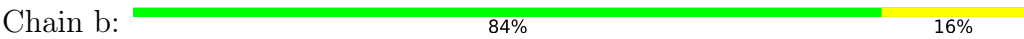
- Molecule 28: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L36



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	51958	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 ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.340	Depositor
Minimum map value	-0.151	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	428.00003, 428.00003, 428.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.40	0/64198	0.41	1/100128 (0.0%)
2	5	0.28	0/2739	0.36	0/4266
3	6	0.19	0/125	0.41	0/194
3	8	0.17	0/188	0.28	0/290
4	A	0.32	0/2150	0.48	0/2888
5	B	0.32	0/1589	0.49	0/2142
6	C	0.30	0/1506	0.43	0/2035
7	D	0.17	0/864	0.47	0/1199
8	E	0.21	0/1346	0.47	0/1818
9	F	0.33	0/1148	0.44	0/1548
10	G	0.32	0/955	0.46	0/1286
11	H	0.32	0/1079	0.54	2/1439 (0.1%)
12	I	0.31	0/1103	0.47	0/1475
13	J	0.34	0/968	0.52	0/1298
14	K	0.22	0/872	0.43	0/1167
15	L	0.29	0/931	0.44	0/1249
16	M	0.35	0/947	0.50	0/1262
17	N	0.30	0/817	0.48	0/1094
18	O	0.31	0/830	0.48	0/1113
19	P	0.27	0/723	0.45	0/967
20	Q	0.23	0/765	0.44	0/1027
21	R	0.28	0/763	0.45	0/1026
22	S	0.31	0/585	0.42	0/783
23	T	0.32	0/641	0.48	0/856
24	U	0.23	0/491	0.49	0/651
25	V	0.30	0/458	0.40	0/612
26	X	0.35	0/453	0.49	0/604
27	Y	0.28	0/433	0.47	0/573
28	Z	0.37	0/366	0.58	0/481
29	a	0.36	0/514	0.52	0/678
30	b	0.30	0/295	0.44	0/389
All	All	0.37	0/90842	0.42	3/136538 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	B	0	1
29	a	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	H	38	LYS	CA-C-N	-6.80	116.38	122.43
11	H	38	LYS	C-N-CA	-6.80	116.38	122.43
1	1	1746	A	C2'-C3'-O3'	5.08	117.13	109.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	B	87	GLU	Peptide
29	a	30	HIS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	57324	0	28814	265	0
2	5	2450	0	1241	18	0
3	6	112	0	56	1	0
3	8	169	0	89	1	0
4	A	2109	0	2175	24	0
5	B	1571	0	1610	19	0
6	C	1485	0	1504	12	0
7	D	865	0	408	3	0
8	E	1327	0	1386	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	F	1122	0	1146	6	0
10	G	945	0	1007	13	0
11	H	1071	0	1141	8	0
12	I	1086	0	1162	10	0
13	J	950	0	998	2	0
14	K	864	0	905	8	0
15	L	919	0	973	5	0
16	M	934	0	997	9	0
17	N	806	0	842	8	0
18	O	825	0	891	8	0
19	P	717	0	777	11	0
20	Q	761	0	811	12	0
21	R	753	0	774	11	0
22	S	577	0	580	3	0
23	T	631	0	667	3	0
24	U	490	0	531	13	0
25	V	453	0	482	2	0
26	X	447	0	435	5	0
27	Y	426	0	462	8	0
28	Z	362	0	401	3	0
29	a	508	0	566	3	0
30	b	294	0	326	3	0
31	1	157	0	0	0	0
31	5	3	0	0	0	0
32	b	1	0	0	0	0
All	All	83514	0	54157	474	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (474) 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)
1:1:1029:A:H61	1:1:1106:G:H1	1.03	0.93
1:1:536:U:O2	1:1:539:G:O6	1.89	0.90
1:1:1954:C:N3	1:1:2591:A:N6	2.19	0.89
1:1:1162:C:O2	1:1:1166:G:N2	2.04	0.89
1:1:1029:A:N6	1:1:1106:G:H1	1.74	0.85
1:1:868:U:H3	1:1:891:A:H61	1.30	0.79
1:1:280:G:N2	1:1:350:C:O2	2.16	0.79
1:1:1162:C:N3	1:1:1166:G:N1	2.26	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:272:U:H3	1:1:359:G:H22	1.31	0.77
1:1:1252:G:OP1	26:X:16:ARG:NH2	2.16	0.77
1:1:1167:U:H2'	1:1:1168:A:H8	1.51	0.76
1:1:1029:A:N1	1:1:1106:G:N2	2.32	0.76
16:M:66:ASN:OD1	16:M:70:ARG:NH1	2.20	0.75
1:1:162:U:O2	1:1:164:C:N4	2.20	0.75
1:1:1328:U:OP2	19:P:81:LYS:NZ	2.20	0.74
11:H:87:VAL:O	11:H:120:ARG:NH2	2.16	0.73
1:1:1014:G:H1	1:1:1130:C:H5	1.35	0.72
25:V:6:VAL:HG12	25:V:56:VAL:HG22	1.71	0.71
1:1:274:A:H2	1:1:356:G:H21	1.38	0.71
8:E:45:GLN:HB3	8:E:50:LEU:HD23	1.72	0.71
8:E:164:TYR:HB2	8:E:167:GLU:HB2	1.73	0.71
30:b:2:LYS:NZ	30:b:32:ARG:O	2.25	0.69
1:1:677:U:O2'	28:Z:5:PHE:O	2.07	0.69
24:U:42:GLU:HA	24:U:45:VAL:HG22	1.75	0.69
4:A:135:MET:O	4:A:167:ARG:NH2	2.26	0.69
1:1:2872:A:OP2	26:X:49:ARG:NH1	2.26	0.68
1:1:2458:A:N6	1:1:2470:G:O2'	2.27	0.67
1:1:1328:U:OP1	19:P:18:LYS:NZ	2.26	0.67
4:A:107:PRO:HD2	4:A:110:LEU:HD22	1.76	0.67
1:1:1271:G:N2	1:1:1274:A:OP2	2.22	0.66
1:1:254:G:N7	29:a:5:LYS:NZ	2.43	0.66
1:1:526:U:O2'	16:M:49:ASP:OD2	2.09	0.66
8:E:94:TYR:HA	8:E:106:ASN:O	1.95	0.66
4:A:123:PRO:O	4:A:128:ASN:ND2	2.29	0.65
27:Y:13:THR:HB	27:Y:38:LYS:HD3	1.76	0.65
1:1:211:U:OP1	28:Z:25:LYS:NZ	2.31	0.64
4:A:6:CYS:SG	4:A:13:ARG:NH2	2.70	0.64
1:1:1472:U:H2'	1:1:1473:A:C8	2.32	0.64
1:1:2501:C:OP2	5:B:131:ARG:NH1	2.30	0.64
5:B:20:GLY:HA2	15:L:82:PRO:HG2	1.80	0.64
1:1:2193:G:OP2	4:A:147:LYS:NZ	2.31	0.64
18:O:74:THR:HB	18:O:107:LYS:HB2	1.80	0.64
1:1:708:C:H3'	1:1:709:A:H8	1.62	0.64
2:5:40:C:N4	7:D:67:VAL:O	2.30	0.63
1:1:892:A:H2'	1:1:893:C:C6	2.34	0.62
1:1:2232:U:H2'	1:1:2233:U:C6	2.34	0.62
7:D:35:THR:O	7:D:154:ILE:HA	2.00	0.62
4:A:125:ARG:HD3	4:A:126:PRO:HD2	1.81	0.62
1:1:1167:U:H2'	1:1:1168:A:C8	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1640:G:O2'	13:J:106:ASP:OD2	2.15	0.61
12:I:19:GLY:O	12:I:39:ARG:NH2	2.34	0.61
10:G:93:PRO:O	10:G:113:LYS:NZ	2.30	0.61
18:O:70:LEU:HD23	18:O:110:VAL:HG13	1.83	0.61
5:B:26:THR:HG21	5:B:196:ILE:HG12	1.83	0.60
6:C:117:LEU:HD11	6:C:187:MET:HE2	1.83	0.60
12:I:33:ALA:HB2	12:I:105:GLU:HG3	1.82	0.60
1:1:273:A:O2'	1:1:274:A:O5'	2.18	0.60
5:B:184:ASP:HB3	5:B:189:VAL:HG12	1.84	0.60
17:N:36:ASP:OD1	17:N:36:ASP:N	2.34	0.59
22:S:56:ASP:OD1	22:S:58:THR:OG1	2.17	0.59
1:1:1002:U:OP2	16:M:70:ARG:NH2	2.36	0.59
1:1:599:A:H2'	1:1:600:A:C8	2.36	0.59
1:1:1404:G:H2'	1:1:1405:C:C6	2.38	0.59
1:1:2317:A:H2'	1:1:2318:A:C8	2.38	0.59
4:A:136:PRO:O	4:A:139:SER:OG	2.19	0.59
1:1:2366:A:H2'	1:1:2367:A:C8	2.39	0.58
1:1:944:G:OP2	12:I:16:ARG:NH2	2.37	0.58
22:S:53:MET:HE3	22:S:57:HIS:ND1	2.19	0.58
1:1:661:A:OP1	11:H:44:LYS:NZ	2.36	0.58
1:1:2280:U:H2'	1:1:2281:G:C8	2.39	0.58
1:1:2182:G:O2'	1:1:2183:U:OP1	2.19	0.58
1:1:259:G:HO2'	1:1:612:A:HO2'	1.40	0.58
1:1:1421:A:H2'	1:1:1422:A:C8	2.39	0.58
1:1:2784:C:H2'	1:1:2785:U:C6	2.39	0.58
12:I:62:GLY:HA3	12:I:107:GLU:O	2.04	0.57
10:G:9:ASP:OD2	10:G:18:ARG:NH1	2.37	0.57
1:1:1166:G:H2'	1:1:1167:U:C6	2.39	0.57
1:1:1166:G:O2'	1:1:1167:U:O4'	2.08	0.57
1:1:2316:A:H2'	1:1:2317:A:C8	2.40	0.57
1:1:475:A:H5''	20:Q:45:LYS:HD2	1.87	0.57
1:1:2647:C:OP1	8:E:160:LYS:NZ	2.34	0.57
23:T:13:VAL:HG22	23:T:29:PHE:HB2	1.86	0.57
1:1:567:U:H2'	1:1:568:G:C8	2.41	0.56
1:1:901:A:H2'	1:1:902:A:C8	2.40	0.56
21:R:13:GLU:C	21:R:15:LYS:H	2.14	0.56
1:1:2056:G:H1	1:1:2432:U:H3	1.53	0.56
8:E:9:VAL:HG22	8:E:50:LEU:HB2	1.87	0.56
8:E:107:LEU:O	8:E:152:ARG:NH2	2.39	0.56
1:1:1588:A:H5''	1:1:1589:A:H5'	1.87	0.56
6:C:137:LEU:HD11	6:C:147:ILE:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1398:U:H2'	1:1:1399:G:O4'	2.06	0.56
1:1:2483:G:H4'	12:I:80:GLU:HG2	1.87	0.55
5:B:181:VAL:HB	5:B:191:VAL:HG23	1.87	0.55
6:C:97:ARG:HD3	6:C:101:ARG:HH11	1.71	0.55
1:1:2573:U:H2'	1:1:2574:U:H2'	1.88	0.55
24:U:3:THR:HB	24:U:52:ARG:HD3	1.88	0.55
1:1:1170:A:H2'	1:1:1171:C:C6	2.41	0.55
19:P:53:GLU:HG2	19:P:90:GLN:HE22	1.72	0.55
1:1:1598:G:H5''	1:1:1599:A:H5'	1.88	0.55
1:1:1726:U:H2'	1:1:1727:G:O4'	2.07	0.54
8:E:11:VAL:HB	8:E:48:GLY:HA2	1.88	0.54
2:5:88:A:N3	2:5:88:A:H2'	2.22	0.54
5:B:182:SER:HB3	5:B:191:VAL:HG22	1.89	0.54
19:P:37:ALA:O	19:P:80:LYS:NZ	2.41	0.54
8:E:44:LYS:O	8:E:51:GLN:HB2	2.07	0.54
10:G:64:ARG:NH2	10:G:99:PHE:O	2.41	0.54
1:1:1806:G:H2'	1:1:1807:U:H5'	1.89	0.54
1:1:1033:C:H2'	1:1:1034:A:C8	2.43	0.54
18:O:23:ASP:OD2	18:O:26:ARG:NH1	2.41	0.54
1:1:1878:A:H2'	1:1:1879:A:C8	2.42	0.54
12:I:30:GLY:N	12:I:105:GLU:OE2	2.36	0.54
1:1:584:U:H2'	1:1:585:U:C6	2.43	0.54
4:A:137:ILE:HD12	4:A:166:GLY:HA2	1.89	0.53
19:P:91:ASP:OD1	19:P:92:VAL:N	2.33	0.53
24:U:4:LYS:H	24:U:4:LYS:HD3	1.73	0.53
2:5:87:U:O2'	2:5:88:A:O4'	2.25	0.53
4:A:183:LYS:HE3	4:A:268:ILE:HD11	1.89	0.53
21:R:84:HIS:HB3	21:R:87:LYS:O	2.08	0.53
1:1:468:G:N1	1:1:471:A:OP2	2.41	0.53
1:1:1161:A:H2'	1:1:1162:C:C6	2.43	0.53
1:1:394:A:H2'	1:1:395:U:O4'	2.09	0.53
1:1:1476:U:H1'	1:1:1490:G:N2	2.24	0.53
2:5:113:A:H2'	2:5:114:G:C8	2.44	0.53
1:1:1404:G:H22	1:1:1573:C:H42	1.57	0.53
17:N:37:ASP:OD1	17:N:37:ASP:N	2.38	0.53
10:G:70:ARG:HD2	10:G:76:VAL:HG13	1.91	0.53
10:G:24:VAL:HA	10:G:39:ILE:HD13	1.91	0.52
24:U:11:VAL:HG12	24:U:60:LYS:HD2	1.90	0.52
14:K:78:ALA:HB2	14:K:109:ALA:HA	1.90	0.52
17:N:64:ILE:HD11	17:N:97:LYS:HB2	1.91	0.52
1:1:1404:G:H2'	1:1:1405:C:H6	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2674:G:OP1	10:G:78:ARG:NH2	2.42	0.52
2:5:33:A:O2'	2:5:34:U:O5'	2.23	0.52
5:B:113:THR:HG23	5:B:205:ILE:HB	1.90	0.52
5:B:127:ARG:HG3	5:B:168:LEU:HD13	1.90	0.52
1:1:2624:U:O2'	5:B:82:GLU:OE2	2.25	0.52
4:A:71:LYS:NZ	4:A:98:ASP:OD1	2.43	0.52
1:1:1673:G:H2'	1:1:1674:U:C6	2.45	0.52
1:1:1768:U:H5	1:1:1773:A:N7	2.06	0.52
1:1:1303:C:O2'	1:1:1380:A:N3	2.41	0.52
2:5:33:A:HO2'	2:5:34:U:P	2.33	0.52
14:K:26:ARG:NH1	14:K:92:ASP:OD2	2.43	0.52
1:1:1463:G:O2'	1:1:1464:U:OP2	2.25	0.52
1:1:1905:A:H3'	1:1:1906:U:C6	2.45	0.52
1:1:847:G:H2'	1:1:848:G:C8	2.44	0.51
1:1:1907:A:O2'	1:1:1908:A:N7	2.36	0.51
1:1:1798:A:H2'	1:1:1799:A:C8	2.46	0.51
2:5:65:A:H8	2:5:67:C:H41	1.57	0.51
3:6:5:G:H3'	3:6:6:G:C8	2.45	0.51
1:1:1791:A:H2'	1:1:1792:A:C8	2.46	0.51
6:C:180:ILE:HG23	11:H:3:LEU:HG	1.92	0.51
1:1:694:U:H2'	1:1:695:G:O4'	2.10	0.51
8:E:72:LEU:O	8:E:76:VAL:HG13	2.11	0.51
1:1:1483:A:H8	1:1:1569:U:O2'	1.93	0.51
1:1:2182:G:HO2'	1:1:2183:U:P	2.33	0.51
1:1:486:G:H4'	18:O:7:LYS:HB2	1.92	0.51
5:B:30:VAL:O	5:B:188:SER:OG	2.24	0.51
24:U:10:SER:OG	24:U:13:GLU:HG3	2.11	0.51
20:Q:94:TYR:O	20:Q:98:GLY:HA2	2.11	0.50
2:5:87:U:H1'	2:5:88:A:C5	2.46	0.50
1:1:1836:A:H1'	1:1:1837:A:N7	2.26	0.50
19:P:78:ASP:OD1	19:P:78:ASP:N	2.35	0.50
1:1:1476:U:H1'	1:1:1490:G:H22	1.76	0.50
2:5:88:A:OP2	12:I:39:ARG:HD2	2.12	0.50
6:C:170:ASP:OD2	6:C:172:THR:OG1	2.29	0.50
14:K:15:THR:O	14:K:19:ILE:HG12	2.11	0.50
1:1:250:G:H2'	1:1:251:A:C8	2.47	0.50
29:a:21:PHE:HE1	29:a:64:ILE:HG22	1.77	0.50
6:C:20:ARG:NH2	6:C:105:GLN:OE1	2.43	0.50
8:E:129:THR:O	8:E:129:THR:OG1	2.30	0.50
1:1:536:U:O2	1:1:539:G:C6	2.65	0.49
24:U:8:GLU:OE2	24:U:8:GLU:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:156:C:H2'	1:1:157:A:C8	2.47	0.49
1:1:1415:A:H2	1:1:1562:A:H62	1.60	0.49
1:1:1785:U:H2'	1:1:1786:C:H6	1.76	0.49
1:1:2063:U:H2'	1:1:2064:U:C6	2.47	0.49
19:P:11:LYS:HA	24:U:29:ARG:HE	1.77	0.49
1:1:712:A:H2'	1:1:713:A:C8	2.48	0.49
24:U:11:VAL:HA	24:U:14:LEU:HD12	1.94	0.49
1:1:1171:C:O2'	1:1:1172:G:OP1	2.23	0.49
1:1:1457:A:H2'	1:1:1458:A:C8	2.47	0.49
1:1:1558:G:OP2	4:A:83:TYR:OH	2.24	0.49
5:B:87:GLU:HG3	5:B:88:ALA:H	1.78	0.49
6:C:147:ILE:HB	6:C:168:VAL:HG22	1.94	0.49
1:1:1955:A:N3	1:1:2581:G:O2'	2.38	0.49
28:Z:24:THR:O	28:Z:28:ARG:HG3	2.13	0.49
1:1:1583:A:H2'	1:1:1584:C:C6	2.48	0.49
20:Q:83:TYR:HE1	20:Q:92:ARG:HG2	1.78	0.49
1:1:572:C:H2'	1:1:573:A:C8	2.48	0.49
4:A:88:THR:HB	4:A:158:ALA:HB2	1.95	0.49
6:C:86:ALA:O	6:C:87:ARG:NH1	2.46	0.49
24:U:37:LEU:HD22	24:U:39:LYS:H	1.77	0.49
1:1:358:U:H4'	1:1:359:G:O5'	2.13	0.48
1:1:775:G:H5'	1:1:776:G:OP1	2.13	0.48
1:1:1785:U:H2'	1:1:1786:C:C6	2.48	0.48
26:X:30:ASP:O	26:X:34:GLY:N	2.31	0.48
1:1:783:A:N3	1:1:2061:C:O2'	2.40	0.48
1:1:1404:G:O2'	1:1:1405:C:O5'	2.28	0.48
4:A:110:LEU:O	4:A:111:ARG:NH1	2.39	0.48
19:P:67:LYS:HB3	19:P:69:PHE:CE2	2.47	0.48
1:1:1710:G:H1'	1:1:1728:A:N6	2.29	0.48
1:1:2777:C:H2'	1:1:2778:C:C6	2.48	0.48
8:E:75:LEU:O	8:E:79:VAL:HG22	2.14	0.48
1:1:356:G:H3'	1:1:357:A:H2'	1.94	0.48
1:1:1033:C:H2'	1:1:1034:A:H8	1.77	0.48
1:1:1627:G:H2'	1:1:1628:A:C8	2.48	0.48
1:1:1483:A:H2'	1:1:1484:A:C8	2.49	0.48
1:1:405:C:H2'	1:1:406:C:C6	2.49	0.48
1:1:1863:C:H2'	1:1:1864:G:O4'	2.14	0.48
19:P:63:LYS:HA	19:P:78:ASP:HB3	1.95	0.48
1:1:500:U:O2'	1:1:501:C:OP1	2.29	0.47
1:1:2014:C:H2'	1:1:2015:U:C6	2.49	0.47
10:G:7:MET:HB3	10:G:18:ARG:HH21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:282:G:H2'	1:1:283:U:C6	2.49	0.47
1:1:2638:C:H2'	1:1:2639:U:H6	1.79	0.47
8:E:115:TYR:OH	8:E:147:GLU:OE1	2.19	0.47
1:1:283:U:H3	1:1:347:A:H61	1.62	0.47
1:1:1171:C:H2'	1:1:1172:G:O4'	2.14	0.47
1:1:2235:G:H2'	1:1:2236:A:C8	2.49	0.47
2:5:112:C:H2'	2:5:113:A:C8	2.50	0.47
1:1:1847:A:H2'	1:1:1848:U:O4'	2.14	0.47
1:1:78:C:H5'	24:U:7:ARG:NH2	2.30	0.47
1:1:323:U:H4'	20:Q:64:HIS:CD2	2.50	0.47
1:1:2543:U:H2'	1:1:2544:U:C6	2.49	0.47
1:1:2729:A:H2'	1:1:2730:A:C8	2.49	0.47
18:O:71:LYS:HB2	18:O:71:LYS:HE2	1.64	0.47
1:1:707:A:H2'	1:1:708:C:O4'	2.15	0.47
1:1:1778:A:H5''	4:A:219:THR:O	2.15	0.47
1:1:2777:C:O2'	1:1:2798:A:N3	2.46	0.47
2:5:113:A:H2'	2:5:114:G:H8	1.79	0.47
20:Q:93:VAL:HG22	20:Q:100:SER:HA	1.96	0.47
8:E:17:VAL:HG23	8:E:45:GLN:HE22	1.80	0.47
12:I:20:LEU:HD23	12:I:99:PRO:HG2	1.96	0.47
1:1:2720:G:H2'	1:1:2721:G:C8	2.50	0.47
1:1:263:U:H2'	1:1:264:C:O4'	2.15	0.46
1:1:2536:A:H2'	1:1:2537:U:C6	2.50	0.46
1:1:356:G:OP2	1:1:357:A:O2'	2.28	0.46
1:1:2836:U:H2'	1:1:2837:G:O4'	2.15	0.46
8:E:54:PRO:HG3	8:E:62:TRP:CE2	2.50	0.46
1:1:1484:A:H2'	1:1:1486:C:C4	2.51	0.46
1:1:1709:U:H2'	1:1:1710:G:O4'	2.15	0.46
1:1:2250:C:OP1	22:S:19:LYS:NZ	2.49	0.46
8:E:43:LEU:HD11	8:E:50:LEU:HD22	1.98	0.46
20:Q:28:SER:OG	20:Q:29:GLU:N	2.47	0.46
29:a:31:ILE:H	29:a:31:ILE:HG13	1.40	0.46
1:1:1872:U:H2'	1:1:1873:G:O4'	2.15	0.46
6:C:150:ASP:OD1	6:C:194:LYS:HD2	2.15	0.46
16:M:86:ALA:HB2	16:M:116:ALA:HB2	1.97	0.46
1:1:954:C:O2'	1:1:2262:A:N3	2.37	0.46
1:1:2834:U:H5''	15:L:55:ASN:O	2.16	0.46
1:1:2873:U:O2'	1:1:2874:U:H5''	2.15	0.46
8:E:73:ASN:O	8:E:77:LYS:HB2	2.15	0.46
12:I:39:ARG:HB3	12:I:99:PRO:HD3	1.97	0.46
1:1:1028:G:H2'	1:1:1029:A:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1175:G:H5'	17:N:83:TYR:CE1	2.51	0.46
1:1:2318:A:H2'	1:1:2319:G:C8	2.51	0.46
1:1:281:U:H2'	1:1:282:G:C8	2.51	0.46
1:1:733:G:H2'	1:1:734:U:C6	2.50	0.46
20:Q:83:TYR:CE1	20:Q:92:ARG:HG2	2.51	0.46
23:T:40:LEU:HD12	23:T:47:VAL:HG21	1.96	0.46
1:1:2028:U:H2'	1:1:2029:G:H8	1.81	0.46
1:1:2075:U:H2'	1:1:2076:G:C8	2.51	0.46
5:B:196:ILE:HD12	5:B:204:VAL:HG11	1.98	0.46
1:1:536:U:C2	1:1:539:G:O6	2.68	0.45
1:1:838:A:H62	1:1:923:U:H3	1.63	0.45
1:1:1304:A:H2'	1:1:1305:G:H8	1.82	0.45
21:R:83:ARG:NH1	21:R:88:ASN:O	2.48	0.45
1:1:730:A:H1'	1:1:731:C:H5	1.80	0.45
1:1:949:A:H2'	1:1:950:A:C8	2.51	0.45
1:1:1779:U:H2'	1:1:1780:A:C5	2.51	0.45
7:D:93:GLY:C	7:D:95:GLN:H	2.23	0.45
11:H:82:SER:HB3	11:H:116:GLY:HA3	1.96	0.45
24:U:11:VAL:HG22	24:U:12:GLU:OE1	2.16	0.45
1:1:836:G:O2'	1:1:837:A:N7	2.43	0.45
20:Q:18:LYS:HB3	20:Q:18:LYS:HE2	1.64	0.45
21:R:76:VAL:HG12	21:R:97:ARG:HA	1.99	0.45
1:1:487:G:O2'	18:O:62:ASN:ND2	2.47	0.45
1:1:2874:U:O4	26:X:39:ARG:NH1	2.49	0.45
8:E:22:ARG:HD3	8:E:22:ARG:HA	1.76	0.45
11:H:91:ILE:O	11:H:96:THR:HG21	2.17	0.45
14:K:78:ALA:HB1	14:K:112:GLY:HA3	1.99	0.45
27:Y:28:GLU:CD	27:Y:28:GLU:H	2.25	0.45
1:1:740:A:H4'	1:1:1259:G:N3	2.31	0.45
1:1:1404:G:HO2'	1:1:1405:C:C5'	2.29	0.45
5:B:13:THR:HG22	5:B:14:ARG:H	1.81	0.45
1:1:1304:A:H2'	1:1:1305:G:C8	2.52	0.45
1:1:1806:G:C2'	1:1:1807:U:H5'	2.47	0.45
10:G:40:LYS:HD2	10:G:57:VAL:HG12	1.99	0.45
16:M:76:TYR:CZ	16:M:80:ILE:HG13	2.52	0.45
1:1:1631:A:H2'	1:1:1632:A:C8	2.52	0.45
1:1:1701:G:H2'	1:1:1702:U:C6	2.51	0.45
1:1:1905:A:H3'	1:1:1906:U:H6	1.82	0.45
10:G:97:ARG:HD3	10:G:99:PHE:HE1	1.82	0.45
4:A:130:LEU:HB2	4:A:135:MET:HE3	1.99	0.45
17:N:57:ALA:O	17:N:58:LYS:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:P:67:LYS:HB3	19:P:69:PHE:CZ	2.51	0.44
1:1:302:G:N2	1:1:304:G:H3'	2.32	0.44
1:1:540:U:O2'	1:1:541:G:OP1	2.29	0.44
1:1:719:G:H4'	4:A:13:ARG:HD2	1.98	0.44
1:1:840:A:H2'	1:1:841:C:C6	2.53	0.44
1:1:983:G:OP1	16:M:50:ARG:NH1	2.50	0.44
1:1:2028:U:H2'	1:1:2029:G:C8	2.51	0.44
1:1:2232:U:H2'	1:1:2233:U:H6	1.79	0.44
25:V:1:MET:O	25:V:2:LYS:HD3	2.17	0.44
1:1:285:U:H2'	1:1:286:U:C6	2.52	0.44
1:1:711:U:H2'	1:1:712:A:C8	2.51	0.44
1:1:52:A:H2'	1:1:53:A:C8	2.52	0.44
1:1:830:U:H2'	1:1:831:C:C6	2.53	0.44
6:C:131:LYS:HA	6:C:131:LYS:HD3	1.72	0.44
15:L:94:ASP:OD2	15:L:114:ARG:NH2	2.50	0.44
18:O:5:THR:HG23	18:O:107:LYS:HG3	1.99	0.44
1:1:1636:G:H5''	1:1:1637:C:H5'	1.99	0.44
2:5:38:U:O2'	2:5:39:U:H5'	2.18	0.44
4:A:135:MET:HE2	4:A:192:ILE:HG13	1.99	0.44
1:1:164:C:H2'	1:1:165:A:O4'	2.18	0.44
5:B:152:ASN:C	5:B:154:THR:H	2.26	0.44
14:K:98:TYR:O	14:K:103:LYS:HB2	2.17	0.44
1:1:92:A:H2'	1:1:93:A:O4'	2.18	0.44
1:1:181:A:H2'	1:1:182:A:C8	2.52	0.44
1:1:990:A:H2'	1:1:991:A:C8	2.52	0.44
1:1:1477:U:H1'	1:1:1489:G:N2	2.33	0.44
1:1:2057:U:H5	1:1:2419:A:N7	2.16	0.44
1:1:1404:G:H4'	1:1:1405:C:OP1	2.18	0.44
1:1:2580:C:H2'	1:1:2581:G:C8	2.52	0.44
8:E:33:LEU:HD13	8:E:75:LEU:HD22	1.98	0.44
27:Y:50:ILE:HG23	27:Y:50:ILE:O	2.18	0.44
1:1:699:G:H2'	1:1:700:U:C6	2.53	0.43
1:1:1018:A:H2'	1:1:1019:A:C8	2.53	0.43
1:1:2792:C:H2'	1:1:2793:C:C6	2.54	0.43
1:1:2262:A:H2'	1:1:2263:A:C8	2.53	0.43
4:A:146:LEU:HD21	4:A:154:LEU:HD11	1.99	0.43
21:R:68:LYS:HB2	21:R:68:LYS:HE2	1.84	0.43
1:1:1472:U:H2'	1:1:1473:A:H8	1.80	0.43
1:1:2692:C:O2'	1:1:2693:C:OP1	2.36	0.43
1:1:175:A:H2'	1:1:176:A:C8	2.52	0.43
1:1:1022:A:H1'	30:b:23:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:59:VAL:HG22	17:N:101:ILE:HG12	1.99	0.43
1:1:12:U:O2	1:1:2615:C:H4'	2.19	0.43
1:1:1349:G:H2'	1:1:1350:C:C6	2.53	0.43
10:G:38:ILE:HD11	10:G:111:PHE:HZ	1.82	0.43
12:I:83:MET:HE2	12:I:83:MET:HA	2.00	0.43
27:Y:6:ARG:HG3	27:Y:50:ILE:HG13	2.01	0.43
1:1:787:C:H2'	1:1:788:U:C6	2.53	0.43
4:A:8:PRO:HB3	4:A:14:ARG:HG3	2.00	0.43
21:R:9:GLN:HG2	21:R:45:THR:HB	2.00	0.43
1:1:680:A:H2'	1:1:681:U:C6	2.53	0.43
1:1:1374:A:H2'	1:1:1375:U:C6	2.54	0.43
1:1:1430:U:H2'	1:1:1431:C:C6	2.54	0.43
11:H:57:THR:O	11:H:62:ARG:NH1	2.51	0.43
1:1:295:A:O5'	20:Q:80:ARG:NH2	2.52	0.43
1:1:816:A:O2'	11:H:56:GLN:OE1	2.29	0.43
1:1:849:G:N3	1:1:2257:A:H2'	2.34	0.43
2:5:33:A:O2'	2:5:34:U:P	2.76	0.43
16:M:58:ARG:HA	16:M:61:TRP:CE3	2.54	0.43
1:1:134:U:H2'	1:1:135:A:C8	2.54	0.43
1:1:471:A:N3	1:1:473:G:H5''	2.34	0.43
8:E:93:GLY:O	8:E:95:LYS:HG2	2.19	0.43
1:1:1030:A:H61	1:1:1105:G:H1	1.67	0.42
4:A:158:ALA:HB1	4:A:197:ASN:HB3	2.01	0.42
8:E:152:ARG:HD2	8:E:152:ARG:HA	1.74	0.42
20:Q:74:THR:OG1	20:Q:75:THR:N	2.52	0.42
1:1:154:A:H2'	1:1:155:A:C8	2.54	0.42
1:1:1435:C:H2'	1:1:1436:U:C6	2.54	0.42
1:1:2522:C:H2'	1:1:2523:A:O4'	2.19	0.42
8:E:55:ALA:O	8:E:56:LYS:HB3	2.18	0.42
15:L:90:LYS:HE2	15:L:90:LYS:HB3	1.74	0.42
1:1:405:C:H2'	1:1:406:C:H6	1.83	0.42
1:1:78:C:H5'	24:U:7:ARG:HH22	1.85	0.42
16:M:48:ARG:HH21	16:M:49:ASP:CG	2.26	0.42
27:Y:5:ILE:HD13	27:Y:21:LYS:HD2	2.00	0.42
2:5:93:U:OP2	21:R:23:ARG:NH1	2.53	0.42
5:B:115:GLN:NE2	5:B:170:ASP:O	2.52	0.42
8:E:9:VAL:HG12	8:E:69:ARG:HE	1.84	0.42
2:5:87:U:H2'	2:5:87:U:O2	2.19	0.42
2:5:91:C:OP1	21:R:26:ARG:NH1	2.52	0.42
8:E:6:LYS:HE2	8:E:62:TRP:CH2	2.55	0.42
24:U:18:LEU:HD11	24:U:54:LYS:HE2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1498:A:H2'	1:1:1499:U:O4'	2.19	0.42
1:1:2280:U:OP1	1:1:2369:U:O2'	2.36	0.42
1:1:2604:U:H1'	26:X:4:GLN:HB3	2.00	0.42
2:5:19:G:H2'	2:5:20:A:C8	2.54	0.42
1:1:2060:A:H2'	1:1:2061:C:C6	2.55	0.42
23:T:78:ILE:HD13	23:T:78:ILE:HA	1.86	0.42
27:Y:23:LYS:HB2	27:Y:23:LYS:HE3	1.74	0.42
1:1:962:A:H3'	1:1:963:A:H2'	2.01	0.42
1:1:2306:C:H2'	1:1:2307:G:C8	2.54	0.42
1:1:2564:C:H5'	5:B:152:ASN:HB2	2.02	0.42
5:B:5:LEU:HD13	5:B:30:VAL:HG11	2.00	0.42
10:G:93:PRO:HG2	10:G:113:LYS:HE2	2.02	0.42
1:1:192:G:O2'	1:1:668:A:N1	2.51	0.42
1:1:577:A:N1	1:1:800:G:O2'	2.48	0.42
9:F:109:LEU:O	9:F:111:LYS:NZ	2.42	0.42
1:1:1366:A:O2'	1:1:1368:G:N7	2.43	0.41
5:B:33:ASN:HB3	5:B:51:VAL:HG13	2.02	0.41
5:B:159:PHE:HB3	9:F:81:PRO:HG3	2.01	0.41
9:F:95:HIS:O	9:F:95:HIS:ND1	2.53	0.41
18:O:80:GLY:HA3	18:O:101:THR:HG22	2.01	0.41
21:R:8:ALA:HB1	21:R:44:VAL:HG13	2.01	0.41
27:Y:15:TYR:HB2	27:Y:38:LYS:HD2	2.01	0.41
1:1:157:A:H2'	1:1:158:U:O4'	2.21	0.41
1:1:2027:G:H2'	1:1:2028:U:O4'	2.20	0.41
1:1:64:G:H2'	1:1:65:C:C6	2.55	0.41
1:1:1434:C:H2'	1:1:1435:C:C6	2.56	0.41
1:1:1470:U:H2'	1:1:1471:G:C8	2.55	0.41
1:1:1912:U:O2'	1:1:1913:C:O5'	2.35	0.41
8:E:26:VAL:CG1	8:E:79:VAL:HG21	2.51	0.41
1:1:456:U:H2'	1:1:457:G:O4'	2.21	0.41
1:1:564:U:O2'	1:1:566:A:OP1	2.27	0.41
1:1:1917:A:H2'	1:1:1918:G:O4'	2.20	0.41
1:1:2295:C:H5''	1:1:2296:G:H2'	2.02	0.41
9:F:28:LEU:HD12	9:F:142:ILE:HG21	2.01	0.41
9:F:114:LEU:HG	9:F:118:MET:HE3	2.03	0.41
20:Q:31:ARG:HA	20:Q:63:LEU:O	2.20	0.41
1:1:303:G:H2'	1:1:304:G:C8	2.55	0.41
1:1:727:C:H2'	1:1:728:C:C6	2.56	0.41
1:1:2566:A:H2'	1:1:2603:A:N6	2.36	0.41
19:P:67:LYS:HD2	19:P:69:PHE:CE1	2.56	0.41
1:1:537:U:H1'	1:1:539:G:N1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1455:G:P	1:1:1537:G:H21	2.44	0.41
1:1:1492:U:H2'	1:1:1493:A:C8	2.55	0.41
1:1:1835:G:O2'	1:1:1836:A:H5'	2.20	0.41
1:1:1836:A:O3'	1:1:1837:A:H8	2.03	0.41
30:b:25:VAL:HB	30:b:35:GLN:HB2	2.02	0.41
1:1:286:U:H2'	1:1:287:U:C6	2.56	0.41
1:1:297:G:H2'	1:1:298:C:H6	1.86	0.41
1:1:1702:U:HO2'	1:1:1703:U:P	2.43	0.41
8:E:35:PHE:CE1	8:E:37:LEU:HG	2.55	0.41
8:E:102:VAL:HG13	8:E:116:ALA:HA	2.03	0.41
1:1:256:A:H2'	1:1:257:C:H6	1.86	0.41
1:1:351:A:H8	1:1:351:A:OP2	2.04	0.41
1:1:1342:A:H2'	1:1:1343:G:O4'	2.21	0.41
1:1:1680:A:H2'	1:1:1681:A:C8	2.55	0.41
1:1:1788:G:OP1	4:A:258:ARG:HD2	2.21	0.41
1:1:1835:G:H2'	1:1:1836:A:C8	2.56	0.41
4:A:29:PRO:HG3	4:A:63:ARG:NH2	2.36	0.41
14:K:66:ASN:HA	14:K:101:ARG:HD3	2.03	0.41
1:1:265:A:H4'	1:1:266:G:OP1	2.19	0.41
1:1:571:U:O3'	16:M:31:VAL:HG13	2.21	0.41
1:1:630:U:H2'	1:1:631:C:C6	2.56	0.41
1:1:706:A:H2'	1:1:707:A:C8	2.56	0.41
1:1:798:U:H1'	1:1:2434:G:OP1	2.21	0.41
1:1:919:G:H2'	1:1:920:U:C6	2.56	0.41
1:1:974:A:N3	1:1:974:A:H2'	2.36	0.41
1:1:1028:G:H2'	1:1:1029:A:H8	1.86	0.41
1:1:2193:G:H2'	1:1:2194:U:C6	2.56	0.41
3:8:69:C:H2'	3:8:70:G:H8	1.86	0.41
6:C:114:GLN:NE2	11:H:2:THR:HG22	2.34	0.41
6:C:129:LYS:HD3	6:C:129:LYS:HA	1.87	0.41
8:E:35:PHE:CE2	8:E:71:VAL:HG21	2.55	0.41
9:F:106:LYS:HE3	9:F:106:LYS:HB3	1.79	0.41
14:K:97:LYS:HG2	14:K:99:HIS:H	1.85	0.41
17:N:81:LYS:HA	17:N:81:LYS:HD3	1.93	0.41
20:Q:37:LEU:HD12	20:Q:37:LEU:HA	1.71	0.41
1:1:804:U:H2'	1:1:805:C:C6	2.56	0.41
1:1:1644:G:C5	13:J:9:LYS:HD2	2.56	0.41
4:A:145:GLU:HG2	4:A:151:GLY:C	2.46	0.41
10:G:40:LYS:HD3	10:G:58:MET:O	2.21	0.41
21:R:13:GLU:C	21:R:15:LYS:N	2.78	0.41
21:R:72:LYS:HA	21:R:72:LYS:HD3	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1734:C:H2'	1:1:1735:G:H5''	2.02	0.40
1:1:2053:C:H2'	1:1:2054:C:C6	2.56	0.40
17:N:42:VAL:HG22	17:N:47:ILE:HG23	2.03	0.40
1:1:937:A:H2'	1:1:938:C:C6	2.55	0.40
1:1:2409:C:H5'	27:Y:50:ILE:HD11	2.03	0.40
1:1:134:U:H2'	1:1:135:A:H8	1.87	0.40
1:1:350:C:O2'	1:1:351:A:H5'	2.21	0.40
1:1:2296:G:H5'	1:1:2297:G:N3	2.36	0.40
8:E:158:LYS:HB3	8:E:158:LYS:HE3	1.79	0.40
1:1:9:A:N1	1:1:2789:U:H5	2.19	0.40
1:1:571:U:H2'	1:1:572:C:C6	2.56	0.40
4:A:106:ALA:O	4:A:196:SER:HB2	2.21	0.40
10:G:77:ILE:HD11	15:L:75:ARG:HE	1.86	0.40
2:5:13:U:O3'	2:5:105:U:O2'	2.38	0.40
14:K:5:LYS:HG3	14:K:8:ARG:HH21	1.87	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	
4	A	270/274 (98%)	259 (96%)	11 (4%)	0	100	100
5	B	209/212 (99%)	197 (94%)	12 (6%)	0	100	100
6	C	197/200 (98%)	185 (94%)	12 (6%)	0	100	100
7	D	174/178 (98%)	144 (83%)	30 (17%)	0	100	100
8	E	173/177 (98%)	155 (90%)	18 (10%)	0	100	100
9	F	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
10	G	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	H	142/146 (97%)	135 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	I	135/137 (98%)	127 (94%)	8 (6%)	0	100	100
13	J	118/125 (94%)	111 (94%)	7 (6%)	0	100	100
14	K	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
15	L	115/122 (94%)	112 (97%)	3 (3%)	0	100	100
16	M	115/119 (97%)	113 (98%)	2 (2%)	0	100	100
17	N	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
18	O	107/110 (97%)	105 (98%)	2 (2%)	0	100	100
19	P	90/106 (85%)	89 (99%)	1 (1%)	0	100	100
20	Q	100/105 (95%)	86 (86%)	14 (14%)	0	100	100
21	R	94/98 (96%)	89 (95%)	5 (5%)	0	100	100
22	S	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
23	T	75/78 (96%)	75 (100%)	0	0	100	100
24	U	59/65 (91%)	55 (93%)	4 (7%)	0	100	100
25	V	55/58 (95%)	53 (96%)	2 (4%)	0	100	100
26	X	52/61 (85%)	50 (96%)	2 (4%)	0	100	100
27	Y	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
28	Z	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
29	a	61/64 (95%)	58 (95%)	2 (3%)	1 (2%)	7	20
30	b	36/38 (95%)	36 (100%)	0	0	100	100
All	All	3016/3136 (96%)	2849 (94%)	166 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	a	31	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	218/220 (99%)	204 (94%)	14 (6%)	16	38
5	B	166/167 (99%)	147 (89%)	19 (11%)	5	14
6	C	145/155 (94%)	142 (98%)	3 (2%)	47	75
8	E	140/142 (99%)	121 (86%)	19 (14%)	3	9
9	F	117/117 (100%)	110 (94%)	7 (6%)	17	41
10	G	103/103 (100%)	92 (89%)	11 (11%)	6	16
11	H	106/108 (98%)	100 (94%)	6 (6%)	18	43
12	I	113/113 (100%)	105 (93%)	8 (7%)	13	33
13	J	97/101 (96%)	94 (97%)	3 (3%)	35	65
14	K	84/85 (99%)	77 (92%)	7 (8%)	10	26
15	L	99/102 (97%)	93 (94%)	6 (6%)	17	40
16	M	85/86 (99%)	84 (99%)	1 (1%)	63	84
17	N	84/84 (100%)	77 (92%)	7 (8%)	10	26
18	O	88/89 (99%)	79 (90%)	9 (10%)	7	18
19	P	78/87 (90%)	70 (90%)	8 (10%)	7	18
20	Q	83/85 (98%)	72 (87%)	11 (13%)	4	10
21	R	78/79 (99%)	76 (97%)	2 (3%)	40	70
22	S	59/64 (92%)	56 (95%)	3 (5%)	21	48
23	T	69/70 (99%)	64 (93%)	5 (7%)	13	32
24	U	53/56 (95%)	45 (85%)	8 (15%)	3	7
25	V	53/54 (98%)	51 (96%)	2 (4%)	29	58
26	X	46/50 (92%)	44 (96%)	2 (4%)	26	54
27	Y	47/47 (100%)	47 (100%)	0	100	100
28	Z	36/36 (100%)	36 (100%)	0	100	100
29	a	52/53 (98%)	49 (94%)	3 (6%)	18	42
30	b	33/33 (100%)	32 (97%)	1 (3%)	36	66
All	All	2332/2386 (98%)	2167 (93%)	165 (7%)	15	33

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	10	SER
4	A	17	GLU
4	A	20	VAL

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Mol	Chain	Res	Type
4	A	22	ASP
4	A	79	GLU
4	A	86	SER
4	A	88	THR
4	A	118	SER
4	A	139	SER
4	A	168	ASP
4	A	170	SER
4	A	186	VAL
4	A	228	ILE
4	A	242	ILE
5	B	13	THR
5	B	15	ILE
5	B	18	ASP
5	B	40	THR
5	B	43	THR
5	B	51	VAL
5	B	53	THR
5	B	59	SER
5	B	63	ASN
5	B	79	LEU
5	B	87	GLU
5	B	101	VAL
5	B	113	THR
5	B	141	VAL
5	B	153	GLN
5	B	171	GLU
5	B	185	THR
5	B	189	VAL
5	B	191	VAL
6	C	56	LYS
6	C	74	SER
6	C	149	THR
8	E	9	VAL
8	E	20	ASN
8	E	24	VAL
8	E	27	LYS
8	E	36	ASN
8	E	37	LEU
8	E	40	LEU
8	E	49	LYS
8	E	52	LEU

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Mol	Chain	Res	Type
8	E	67	THR
8	E	76	VAL
8	E	81	GLU
8	E	86	LYS
8	E	129	THR
8	E	133	LEU
8	E	160	LYS
8	E	168	VAL
8	E	170	LEU
8	E	175	LYS
9	F	4	LEU
9	F	60	GLU
9	F	62	VAL
9	F	64	VAL
9	F	70	LEU
9	F	141	ASP
9	F	142	ILE
10	G	29	HIS
10	G	34	SER
10	G	45	GLU
10	G	47	ILE
10	G	51	ARG
10	G	73	ASP
10	G	75	SER
10	G	76	VAL
10	G	80	ASP
10	G	102	VAL
10	G	108	THR
11	H	29	VAL
11	H	117	GLU
11	H	119	THR
11	H	123	THR
11	H	137	ILE
11	H	145	GLU
12	I	57	ARG
12	I	58	ILE
12	I	79	LEU
12	I	80	GLU
12	I	82	ARG
12	I	124	LYS
12	I	132	VAL
12	I	136	VAL

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Mol	Chain	Res	Type
13	J	6	SER
13	J	34	ILE
13	J	89	GLU
14	K	15	THR
14	K	27	LEU
14	K	44	ASP
14	K	58	SER
14	K	61	SER
14	K	99	HIS
14	K	107	ASP
15	L	7	LEU
15	L	15	GLN
15	L	68	SER
15	L	73	VAL
15	L	109	LYS
15	L	115	GLU
16	M	112	LYS
17	N	2	TYR
17	N	32	THR
17	N	33	ILE
17	N	34	THR
17	N	36	ASP
17	N	37	ASP
17	N	99	THR
18	O	5	THR
18	O	8	LEU
18	O	29	SER
18	O	30	VAL
18	O	54	SER
18	O	74	THR
18	O	98	THR
18	O	108	VAL
18	O	110	VAL
19	P	17	GLU
19	P	44	LYS
19	P	52	VAL
19	P	55	VAL
19	P	66	THR
19	P	78	ASP
19	P	86	LEU
19	P	92	VAL
20	Q	28	SER

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Mol	Chain	Res	Type
20	Q	40	VAL
20	Q	57	VAL
20	Q	58	THR
20	Q	60	GLU
20	Q	62	SER
20	Q	66	SER
20	Q	70	ILE
20	Q	74	THR
20	Q	79	ASP
20	Q	100	SER
21	R	30	VAL
21	R	44	VAL
22	S	9	SER
22	S	10	THR
22	S	32	THR
23	T	19	SER
23	T	22	ASN
23	T	24	LYS
23	T	25	THR
23	T	27	ARG
24	U	4	LYS
24	U	11	VAL
24	U	17	LEU
24	U	29	ARG
24	U	32	LYS
24	U	34	THR
24	U	37	LEU
24	U	47	ARG
25	V	4	ILE
25	V	57	GLU
26	X	44	LYS
26	X	53	LEU
29	a	30	HIS
29	a	31	ILE
29	a	64	ILE
30	b	6	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	142	HIS
4	A	153	GLN

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Mol	Chain	Res	Type
4	A	250	GLN
5	B	129	ASN
5	B	133	GLN
5	B	143	HIS
6	C	93	GLN
8	E	19	GLN
8	E	45	GLN
8	E	106	ASN
9	F	58	ASN
10	G	29	HIS
12	I	13	HIS
12	I	22	HIS
12	I	46	GLN
15	L	5	HIS
15	L	15	GLN
15	L	44	GLN
17	N	12	HIS
17	N	43	ASN
17	N	69	HIS
19	P	2	ASN
19	P	90	GLN
20	Q	43	HIS
22	S	29	GLN
23	T	6	GLN
23	T	34	HIS
23	T	36	HIS
24	U	44	GLN
26	X	6	ASN
26	X	25	ASN
26	X	37	HIS
30	b	35	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2666/2903 (91%)	452 (16%)	16 (0%)
2	5	114/117 (97%)	23 (20%)	3 (2%)
3	6	4/77 (5%)	2 (50%)	0
3	8	7/77 (9%)	3 (42%)	0
All	All	2791/3174 (87%)	480 (17%)	19 (0%)

All (480) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	15	G
1	1	34	U
1	1	46	G
1	1	58	G
1	1	60	G
1	1	62	U
1	1	63	A
1	1	71	A
1	1	74	A
1	1	75	G
1	1	85	G
1	1	94	U
1	1	96	U
1	1	97	C
1	1	100	U
1	1	118	A
1	1	119	A
1	1	120	U
1	1	137	U
1	1	140	A
1	1	142	G
1	1	165	A
1	1	196	A
1	1	213	A
1	1	215	G
1	1	216	A
1	1	221	A
1	1	222	A
1	1	225	C
1	1	229	U
1	1	230	G
1	1	233	A
1	1	248	G
1	1	261	G
1	1	264	C
1	1	265	A
1	1	266	G
1	1	268	C
1	1	271	U
1	1	272	U
1	1	274	A
1	1	280	G
1	1	297	G

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Mol	Chain	Res	Type
1	1	303	G
1	1	306	A
1	1	324	G
1	1	325	A
1	1	328	U
1	1	347	A
1	1	348	C
1	1	349	A
1	1	350	C
1	1	351	A
1	1	352	U
1	1	353	A
1	1	357	A
1	1	358	U
1	1	359	G
1	1	361	C
1	1	363	A
1	1	364	G
1	1	378	G
1	1	381	A
1	1	388	G
1	1	395	U
1	1	398	G
1	1	403	G
1	1	404	A
1	1	416	G
1	1	428	C
1	1	448	C
1	1	449	A
1	1	469	A
1	1	473	G
1	1	482	U
1	1	486	G
1	1	488	G
1	1	495	A
1	1	497	A
1	1	500	U
1	1	501	C
1	1	520	A
1	1	522	G
1	1	523	C
1	1	524	A

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Mol	Chain	Res	Type
1	1	528	G
1	1	537	U
1	1	538	U
1	1	539	G
1	1	540	U
1	1	541	G
1	1	554	A
1	1	564	U
1	1	566	A
1	1	568	G
1	1	577	A
1	1	594	A
1	1	600	A
1	1	604	U
1	1	605	A
1	1	606	U
1	1	618	A
1	1	626	C
1	1	628	A
1	1	637	A
1	1	638	G
1	1	644	U
1	1	646	A
1	1	677	U
1	1	701	U
1	1	717	G
1	1	721	A
1	1	729	C
1	1	731	C
1	1	738	U
1	1	755	A
1	1	756	C
1	1	766	G
1	1	767	G
1	1	773	A
1	1	775	G
1	1	776	G
1	1	780	A
1	1	783	A
1	1	785	G
1	1	793	A
1	1	796	G

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Mol	Chain	Res	Type
1	1	803	C
1	1	810	A
1	1	818	U
1	1	819	U
1	1	820	A
1	1	821	G
1	1	837	A
1	1	838	A
1	1	850	G
1	1	857	A
1	1	901	A
1	1	921	A
1	1	922	C
1	1	923	U
1	1	931	A
1	1	936	G
1	1	951	C
1	1	964	G
1	1	972	C
1	1	973	A
1	1	985	C
1	1	986	A
1	1	989	U
1	1	995	C
1	1	999	A
1	1	1002	U
1	1	1003	C
1	1	1012	G
1	1	1016	G
1	1	1023	U
1	1	1024	G
1	1	1032	G
1	1	1102	G
1	1	1106	G
1	1	1118	G
1	1	1122	U
1	1	1124	A
1	1	1125	C
1	1	1126	G
1	1	1132	A
1	1	1134	A
1	1	1161	A

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Mol	Chain	Res	Type
1	1	1164	U
1	1	1165	U
1	1	1168	A
1	1	1170	A
1	1	1171	C
1	1	1172	G
1	1	1194	G
1	1	1226	G
1	1	1235	A
1	1	1236	G
1	1	1238	G
1	1	1241	A
1	1	1244	G
1	1	1254	G
1	1	1256	A
1	1	1259	G
1	1	1260	A
1	1	1274	A
1	1	1288	A
1	1	1289	A
1	1	1290	A
1	1	1302	C
1	1	1309	A
1	1	1317	U
1	1	1333	C
1	1	1334	G
1	1	1340	U
1	1	1353	A
1	1	1356	G
1	1	1367	U
1	1	1368	G
1	1	1371	A
1	1	1374	A
1	1	1376	G
1	1	1383	A
1	1	1396	U
1	1	1397	G
1	1	1404	G
1	1	1405	C
1	1	1406	G
1	1	1407	A
1	1	1415	A

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Mol	Chain	Res	Type
1	1	1416	C
1	1	1417	G
1	1	1421	A
1	1	1440	G
1	1	1446	U
1	1	1449	C
1	1	1455	G
1	1	1456	A
1	1	1463	G
1	1	1470	U
1	1	1478	A
1	1	1482	A
1	1	1484	A
1	1	1485	U
1	1	1493	A
1	1	1496	C
1	1	1497	U
1	1	1498	A
1	1	1500	G
1	1	1504	A
1	1	1550	U
1	1	1557	A
1	1	1560	A
1	1	1569	U
1	1	1573	C
1	1	1575	U
1	1	1576	C
1	1	1580	U
1	1	1581	A
1	1	1586	G
1	1	1587	G
1	1	1599	A
1	1	1601	A
1	1	1607	A
1	1	1630	C
1	1	1638	U
1	1	1639	U
1	1	1641	A
1	1	1652	C
1	1	1665	G
1	1	1686	G
1	1	1698	G

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Mol	Chain	Res	Type
1	1	1703	U
1	1	1705	U
1	1	1706	U
1	1	1711	A
1	1	1727	G
1	1	1728	A
1	1	1729	G
1	1	1735	G
1	1	1736	A
1	1	1737	C
1	1	1745	G
1	1	1747	A
1	1	1753	G
1	1	1762	A
1	1	1765	G
1	1	1776	A
1	1	1777	C
1	1	1789	C
1	1	1790	A
1	1	1791	A
1	1	1797	A
1	1	1800	G
1	1	1805	C
1	1	1807	U
1	1	1818	A
1	1	1836	A
1	1	1837	A
1	1	1853	U
1	1	1858	G
1	1	1859	U
1	1	1860	A
1	1	1861	A
1	1	1862	G
1	1	1865	A
1	1	1894	C
1	1	1895	G
1	1	1896	G
1	1	1902	A
1	1	1903	C
1	1	1904	U
1	1	1905	A
1	1	1913	C

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Mol	Chain	Res	Type
1	1	1916	A
1	1	1918	G
1	1	1919	G
1	1	1926	A
1	1	1927	A
1	1	1929	U
1	1	1944	U
1	1	1952	U
1	1	1953	G
1	1	1956	C
1	1	1959	A
1	1	1960	U
1	1	1961	G
1	1	1980	U
1	1	1982	U
1	1	1986	C
1	1	2010	A
1	1	2011	U
1	1	2012	C
1	1	2016	G
1	1	2017	U
1	1	2018	G
1	1	2019	A
1	1	2020	A
1	1	2022	A
1	1	2025	C
1	1	2032	C
1	1	2044	C
1	1	2045	G
1	1	2049	A
1	1	2050	G
1	1	2051	A
1	1	2058	G
1	1	2061	C
1	1	2086	U
1	1	2182	G
1	1	2183	U
1	1	2187	A
1	1	2193	G
1	1	2200	G
1	1	2201	A
1	1	2212	G

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Mol	Chain	Res	Type
1	1	2214	A
1	1	2227	G
1	1	2228	G
1	1	2240	G
1	1	2257	A
1	1	2268	G
1	1	2272	U
1	1	2276	A
1	1	2277	A
1	1	2287	A
1	1	2294	U
1	1	2296	G
1	1	2297	G
1	1	2298	A
1	1	2307	G
1	1	2309	A
1	1	2311	A
1	1	2314	A
1	1	2316	A
1	1	2336	C
1	1	2339	C
1	1	2347	A
1	1	2370	A
1	1	2372	G
1	1	2373	U
1	1	2374	C
1	1	2380	G
1	1	2385	G
1	1	2391	U
1	1	2392	C
1	1	2395	U
1	1	2408	U
1	1	2411	C
1	1	2412	U
1	1	2414	A
1	1	2415	A
1	1	2418	G
1	1	2419	A
1	1	2421	A
1	1	2424	A
1	1	2430	U
1	1	2434	G

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Mol	Chain	Res	Type
1	1	2437	A
1	1	2459	G
1	1	2463	U
1	1	2465	A
1	1	2467	A
1	1	2469	C
1	1	2480	U
1	1	2487	C
1	1	2491	G
1	1	2492	A
1	1	2494	G
1	1	2507	A
1	1	2509	C
1	1	2518	G
1	1	2531	A
1	1	2536	A
1	1	2543	U
1	1	2545	C
1	1	2555	A
1	1	2556	G
1	1	2562	C
1	1	2563	G
1	1	2571	G
1	1	2591	A
1	1	2592	G
1	1	2597	G
1	1	2598	U
1	1	2602	U
1	1	2604	U
1	1	2618	U
1	1	2635	C
1	1	2650	G
1	1	2652	G
1	1	2658	G
1	1	2660	G
1	1	2678	U
1	1	2679	A
1	1	2693	C
1	1	2697	C
1	1	2703	G
1	1	2715	U
1	1	2718	U

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Mol	Chain	Res	Type
1	1	2722	A
1	1	2733	G
1	1	2737	A
1	1	2746	A
1	1	2754	A
1	1	2755	G
1	1	2766	G
1	1	2767	A
1	1	2769	A
1	1	2770	A
1	1	2783	A
1	1	2785	U
1	1	2786	U
1	1	2787	U
1	1	2789	U
1	1	2794	U
1	1	2797	A
1	1	2800	G
1	1	2807	U
1	1	2809	G
1	1	2810	A
1	1	2824	A
1	1	2838	G
1	1	2850	U
1	1	2856	A
1	1	2862	A
1	1	2869	C
1	1	2873	U
1	1	2875	G
1	1	2890	C
1	1	2891	U
2	5	3	C
2	5	4	U
2	5	5	G
2	5	13	U
2	5	17	A
2	5	23	G
2	5	24	A
2	5	25	A
2	5	29	C
2	5	34	U
2	5	40	C

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Mol	Chain	Res	Type
2	5	50	G
2	5	53	G
2	5	55	G
2	5	63	U
2	5	66	G
2	5	88	A
2	5	97	A
2	5	105	U
2	5	106	C
2	5	107	A
2	5	108	U
2	5	116	U
3	6	3	C
3	6	6	G
3	8	70	G
3	8	75	C
3	8	76	A

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	358	U
1	1	538	U
1	1	567	U
1	1	645	U
1	1	775	G
1	1	1170	A
1	1	1171	C
1	1	1367	U
1	1	1404	G
1	1	1575	U
1	1	1702	U
1	1	1746	A
1	1	2182	G
1	1	2414	A
1	1	2692	C
1	1	2745	U
2	5	4	U
2	5	33	A
2	5	88	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 161 ligands modelled in this entry, 161 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

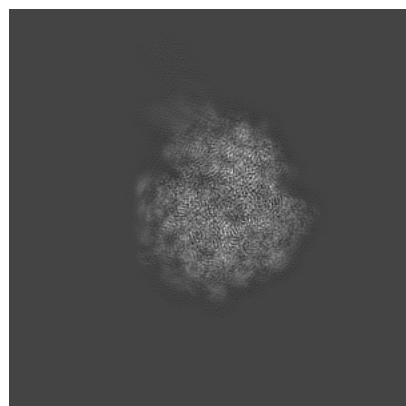
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10809. These allow visual inspection of the internal detail of the map and identification of artifacts.

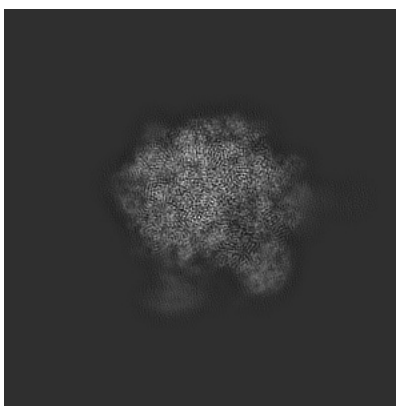
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

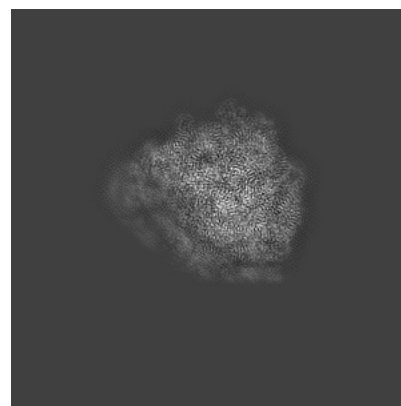
6.1.1 Primary map



X

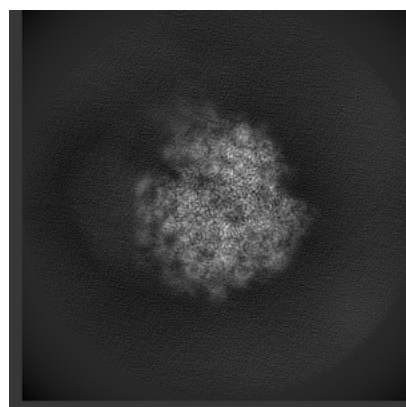


Y

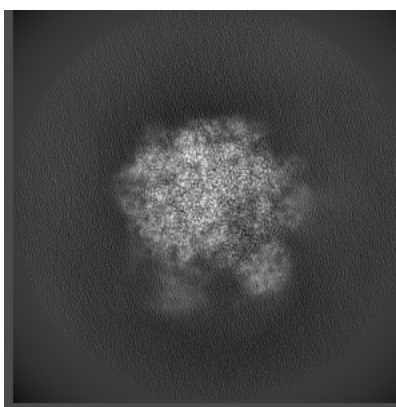


Z

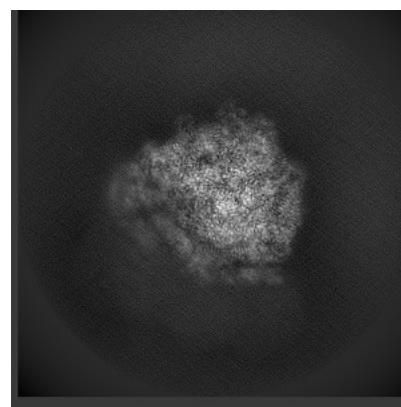
6.1.2 Raw map



X



Y

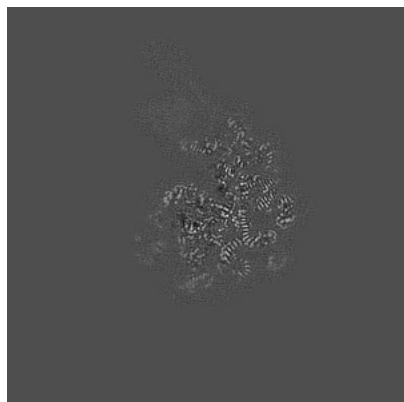


Z

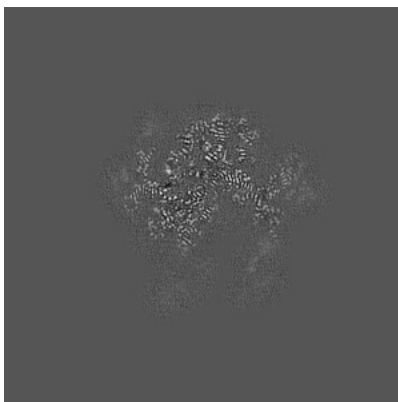
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

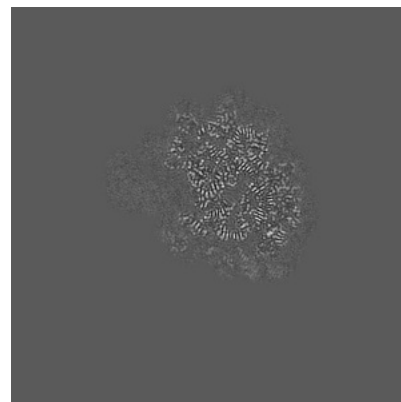
6.2.1 Primary map



X Index: 200

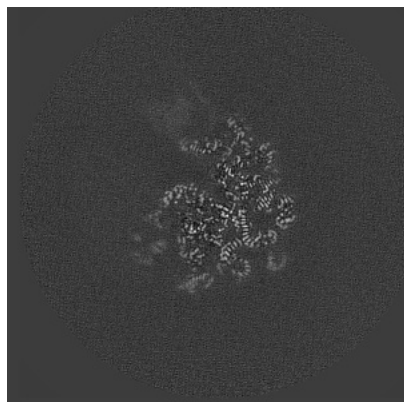


Y Index: 200

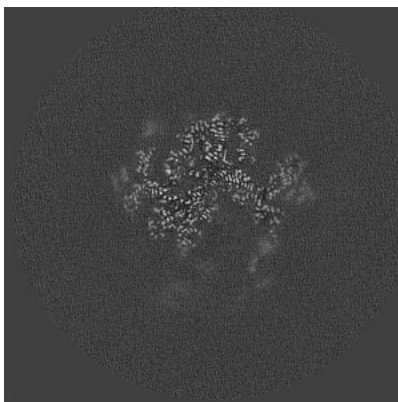


Z Index: 200

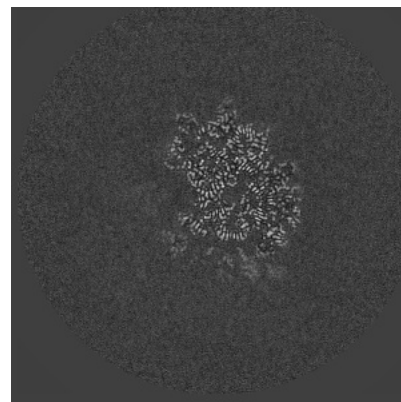
6.2.2 Raw map



X Index: 200



Y Index: 200

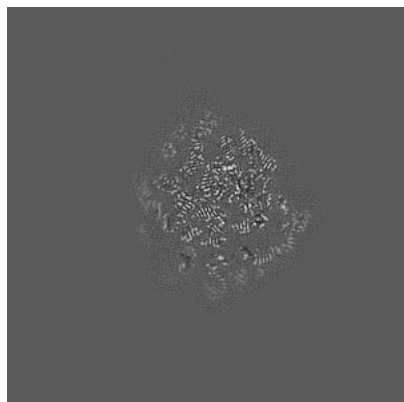


Z Index: 200

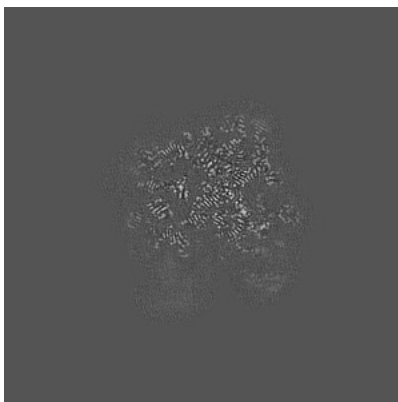
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

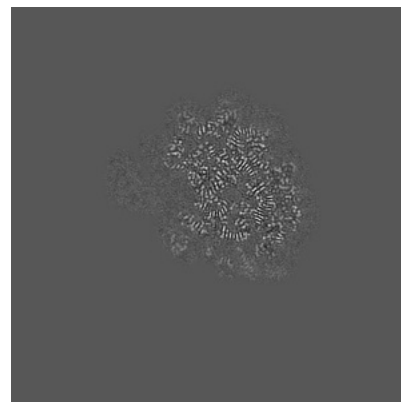
6.3.1 Primary map



X Index: 232

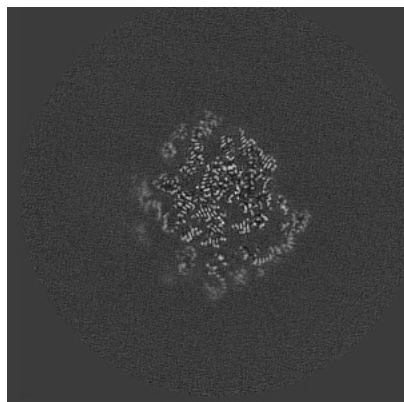


Y Index: 223



Z Index: 201

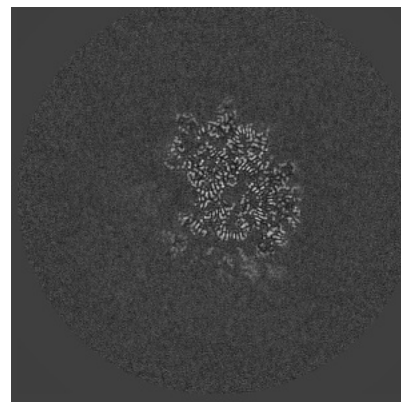
6.3.2 Raw map



X Index: 232



Y Index: 219

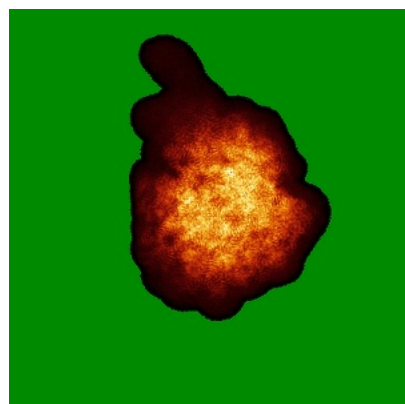


Z Index: 200

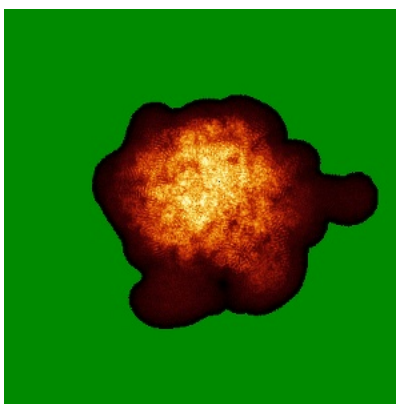
The images above show the largest variance slices of the map in three orthogonal directions.

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

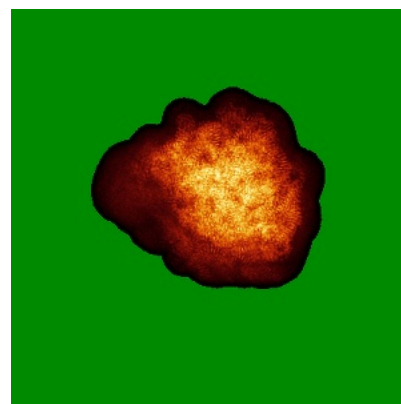
6.4.1 Primary map



X

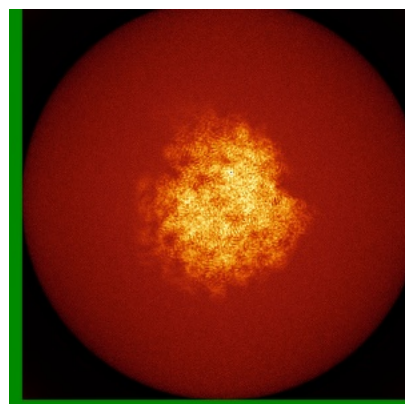


Y

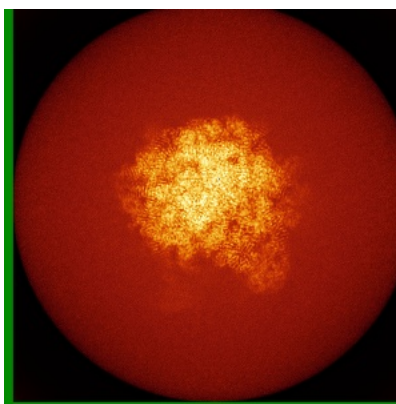


Z

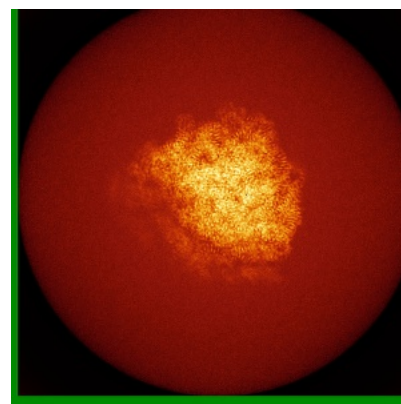
6.4.2 Raw map



X



Y

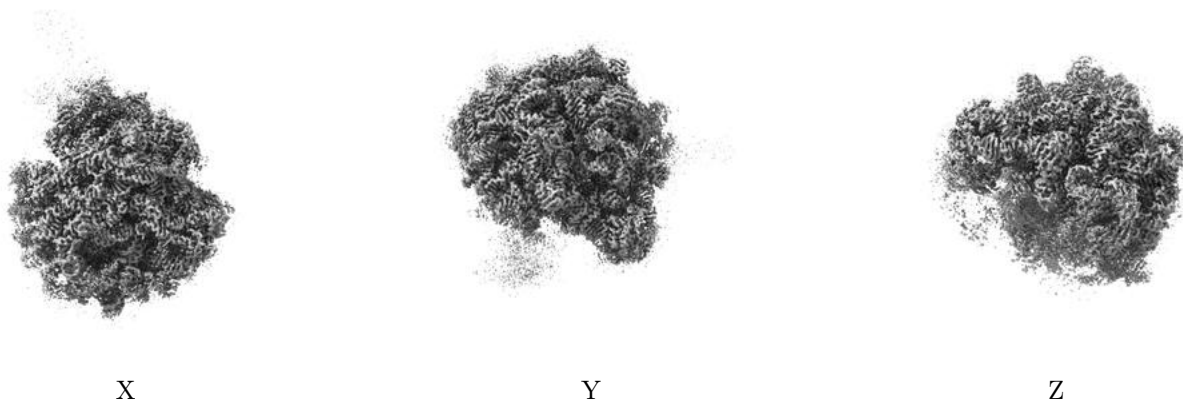


Z

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.

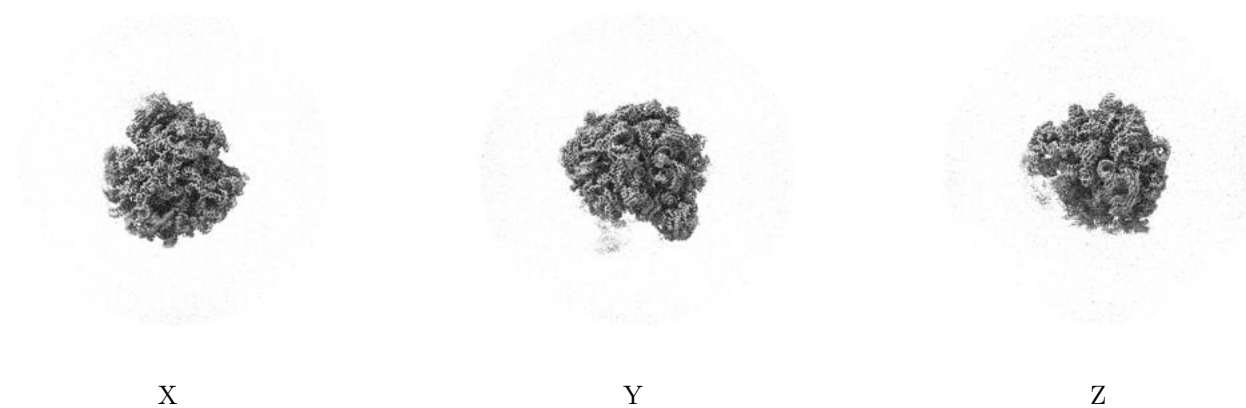
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.

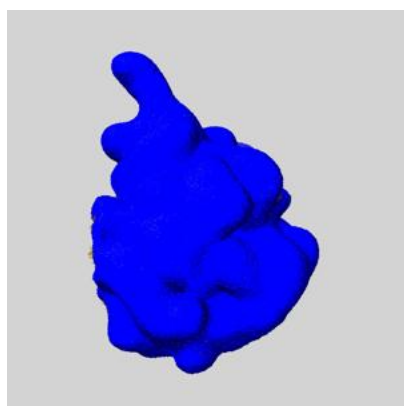
6.6 Mask visualisation [i](#)

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

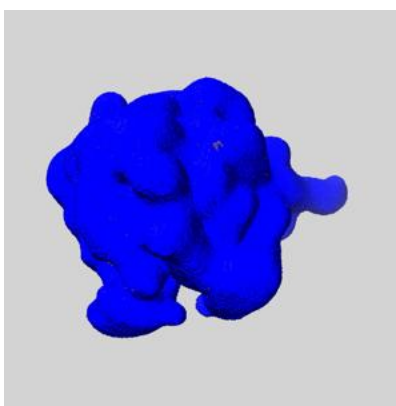
A mask typically either:

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

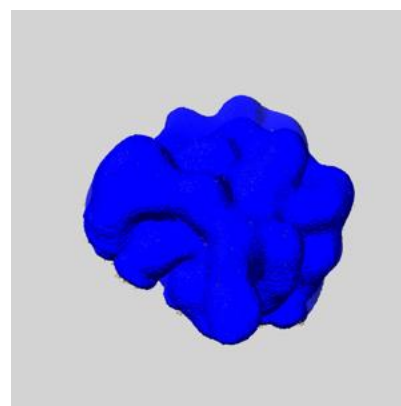
6.6.1 emd_10809_msk_1.map [i](#)



X



Y

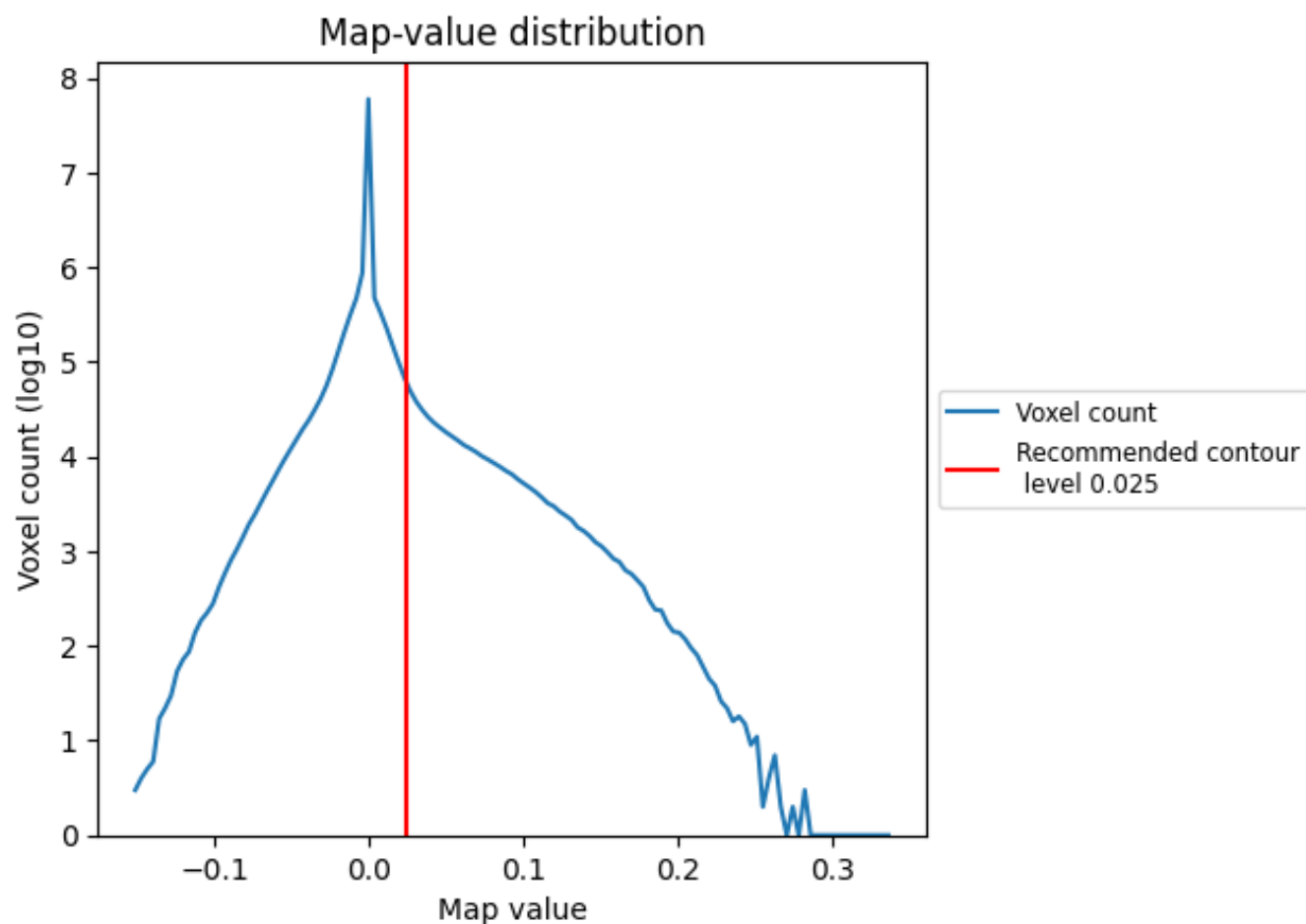


Z

7 Map analysis [i](#)

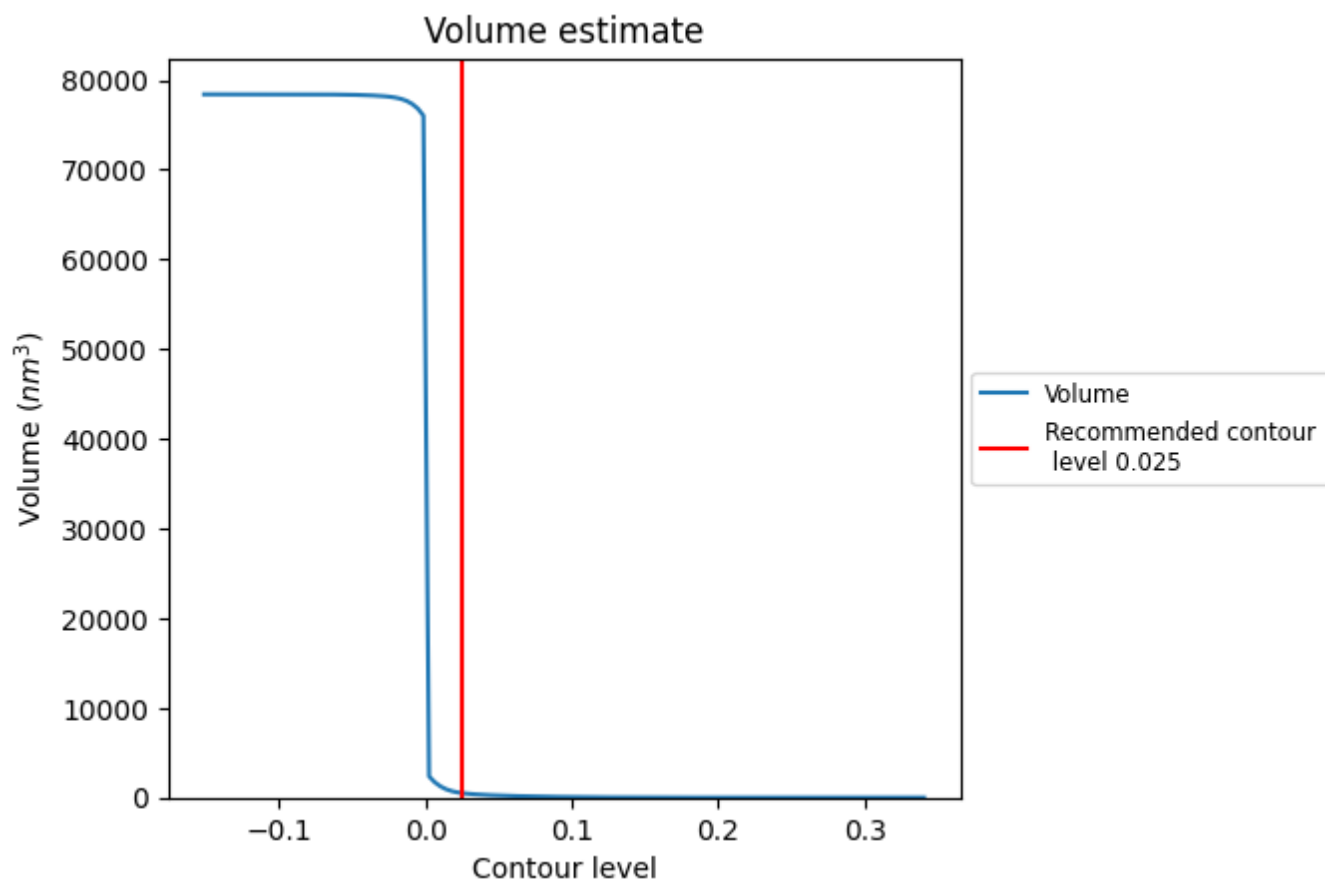
This section contains the results of statistical analysis of the map.

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.

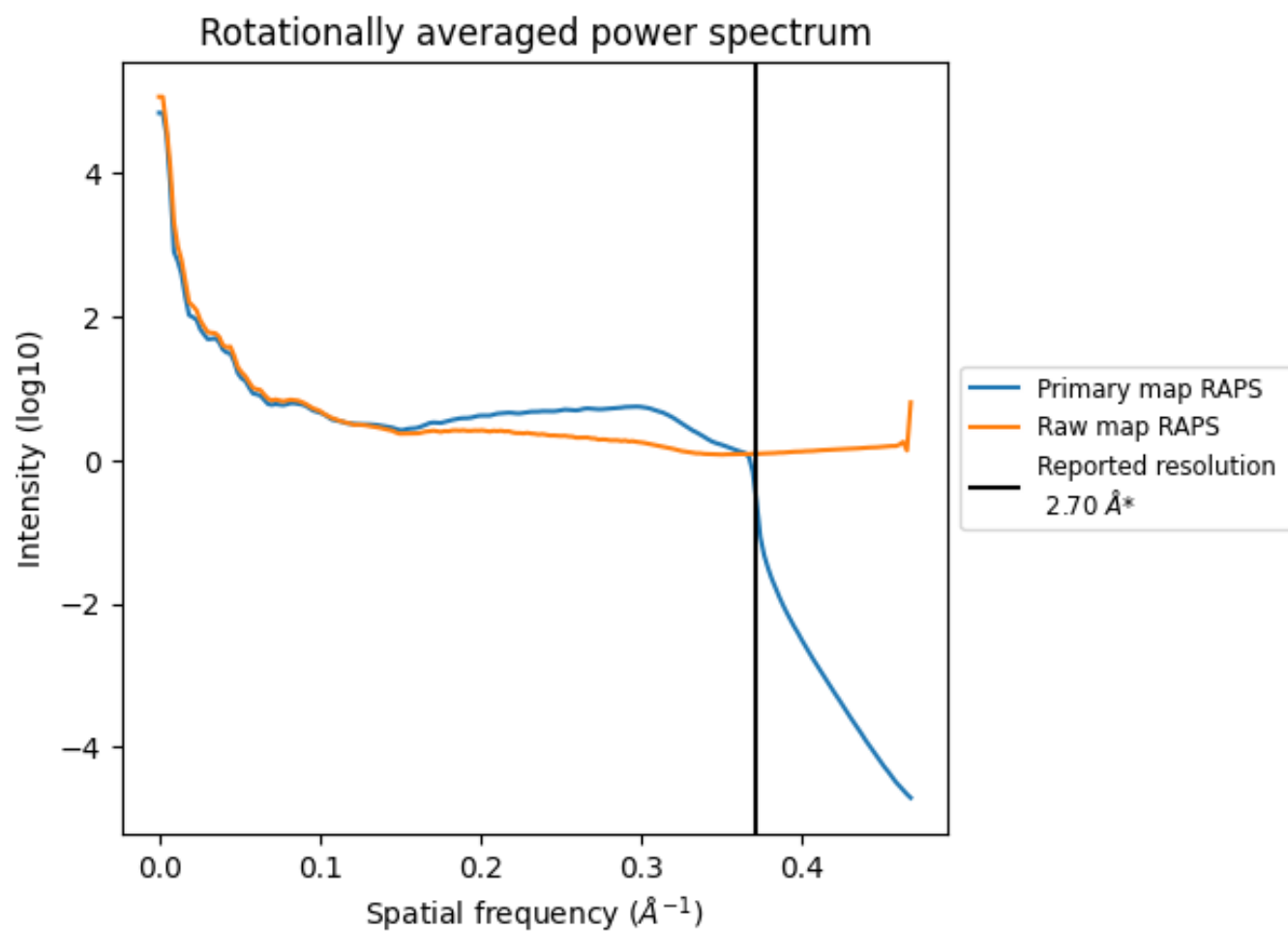
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 500 nm^3 ; this corresponds to an approximate mass of 452 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 ⓘ

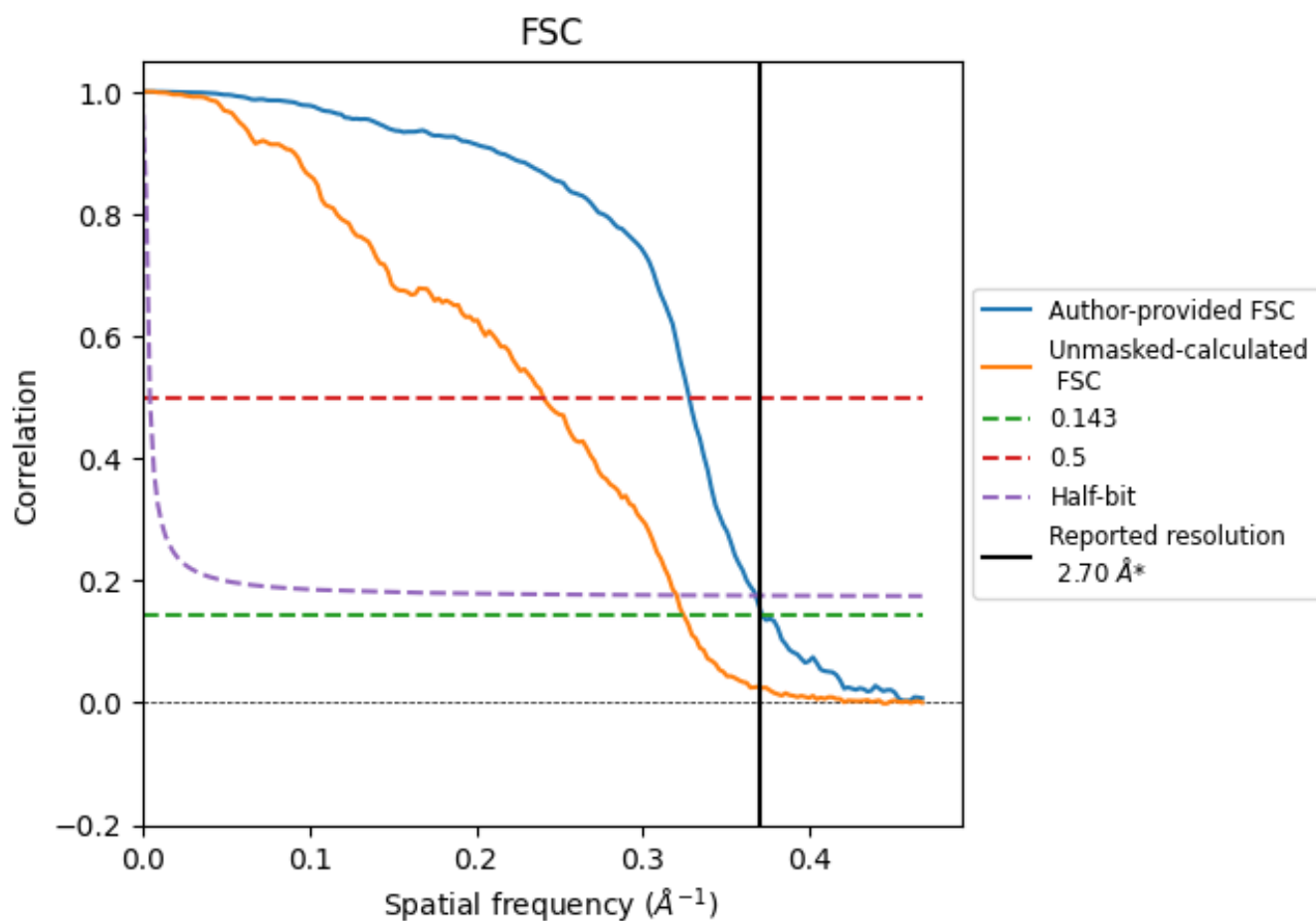


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

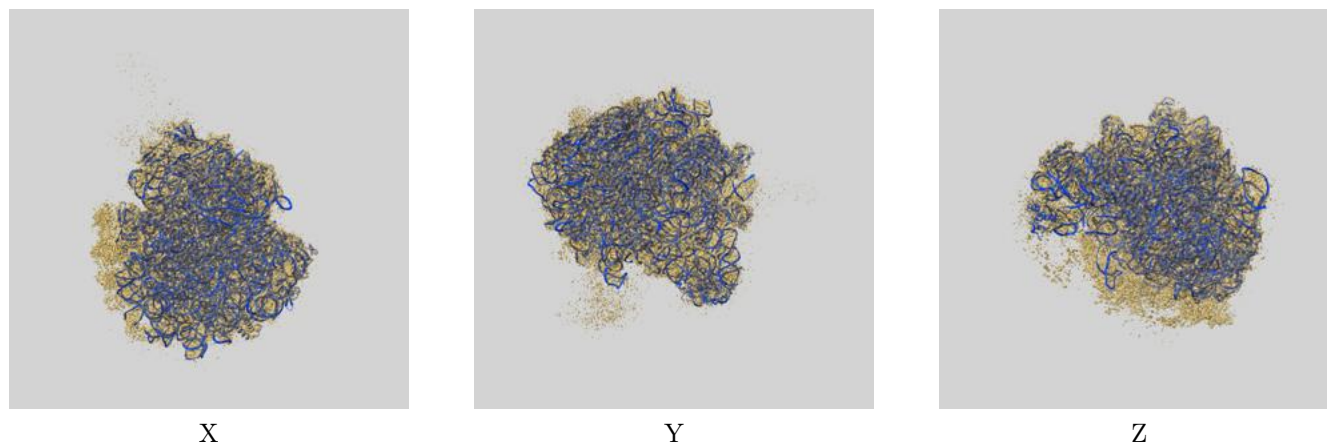
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.69	3.05	2.72
Unmasked-calculated*	3.08	4.16	3.12

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.08 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

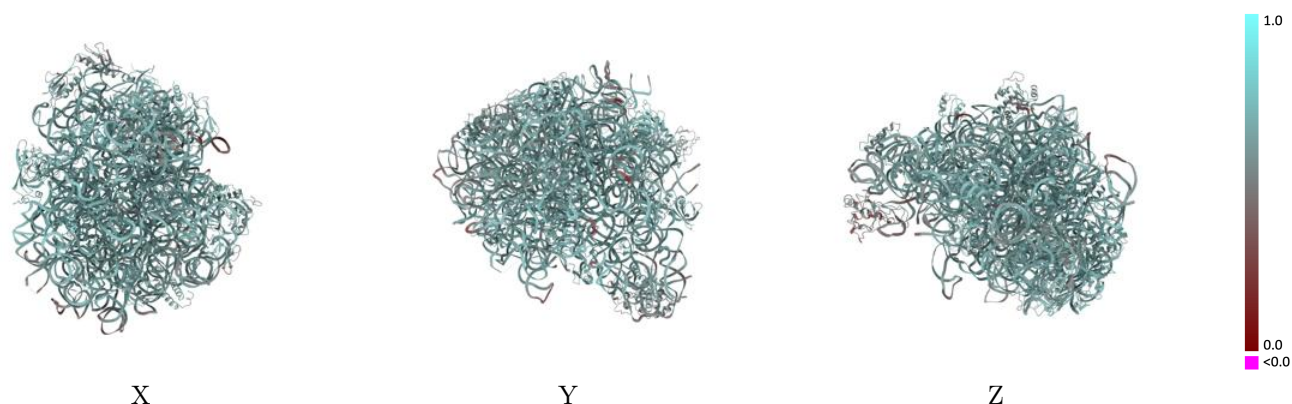
This section contains information regarding the fit between EMDB map EMD-10809 and PDB model 6YHS. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



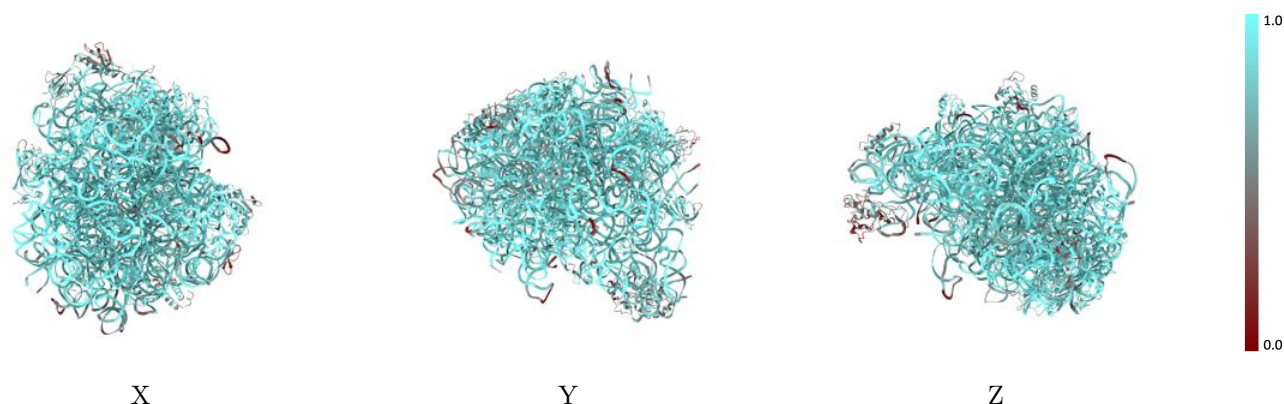
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



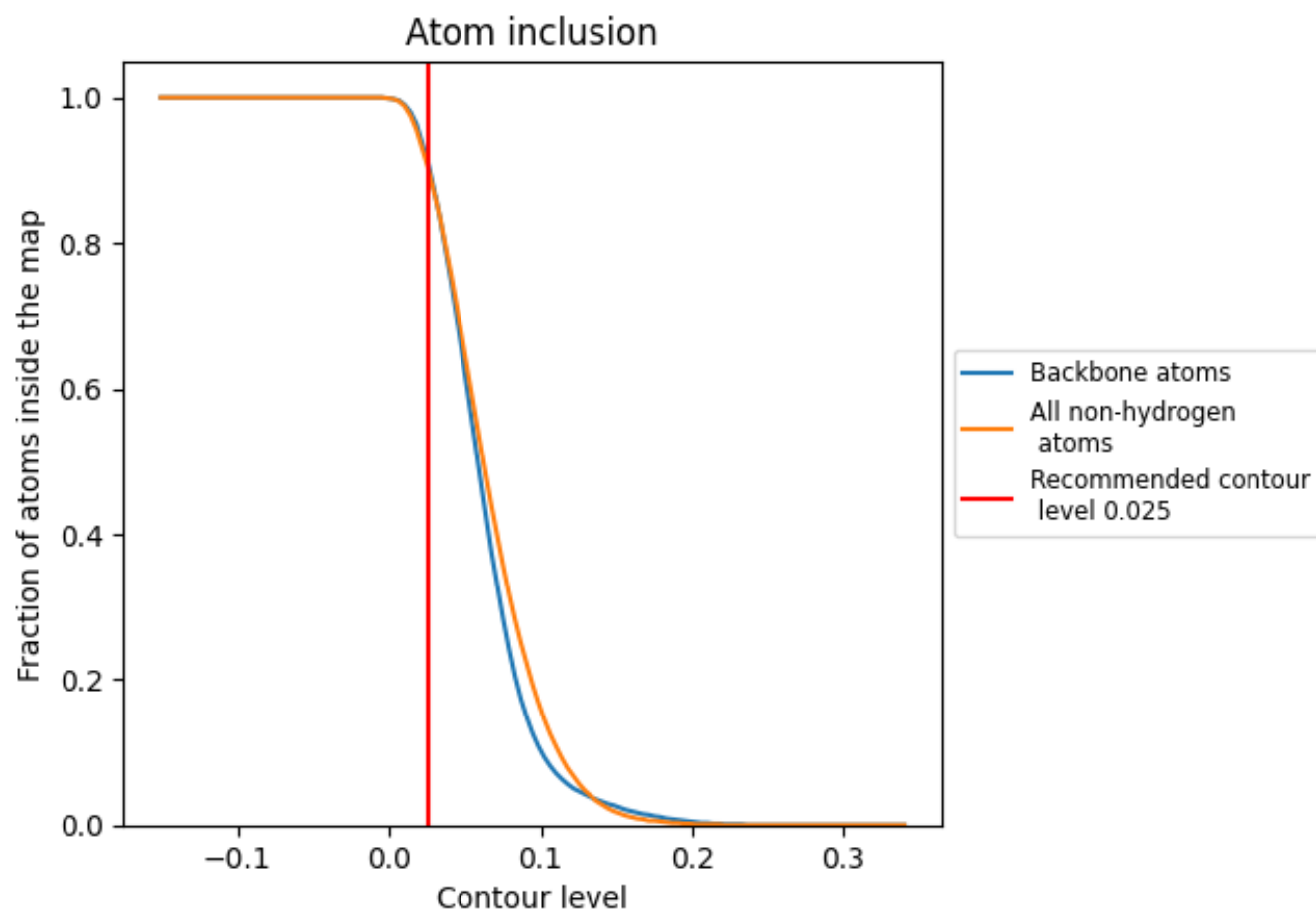
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9090	 0.6390
1	 0.9410	 0.6430
5	 0.8440	 0.5840
6	 0.1610	 0.4920
8	 0.3370	 0.5070
A	 0.9230	 0.6660
B	 0.9260	 0.6600
C	 0.8460	 0.6350
D	 0.4350	 0.4650
E	 0.5940	 0.5670
F	 0.9250	 0.6610
G	 0.8860	 0.6490
H	 0.9000	 0.6520
I	 0.8940	 0.6480
J	 0.9600	 0.6690
K	 0.7420	 0.5980
L	 0.8530	 0.6470
M	 0.9560	 0.6720
N	 0.8920	 0.6470
O	 0.9110	 0.6630
P	 0.7900	 0.6260
Q	 0.6020	 0.5730
R	 0.8140	 0.6360
S	 0.9400	 0.6750
T	 0.8940	 0.6530
U	 0.6350	 0.5730
V	 0.9120	 0.6470
X	 0.8920	 0.6520
Y	 0.8080	 0.6410
Z	 0.9620	 0.6750
a	 0.9770	 0.6770
b	 0.8880	 0.6480

