



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 03:14 PM UTC

PDB ID : 6S0K / pdb_00006s0k
EMDB ID : EMD-10073
Title : Ribosome nascent chain in complex with SecA
Authors : Jomaa, A.; Wang, S.; Shan, S.; Ban, N.
Deposited on : 2019-06-17
Resolution : 3.10 Å (reported)
Based on initial model : 5GAG

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

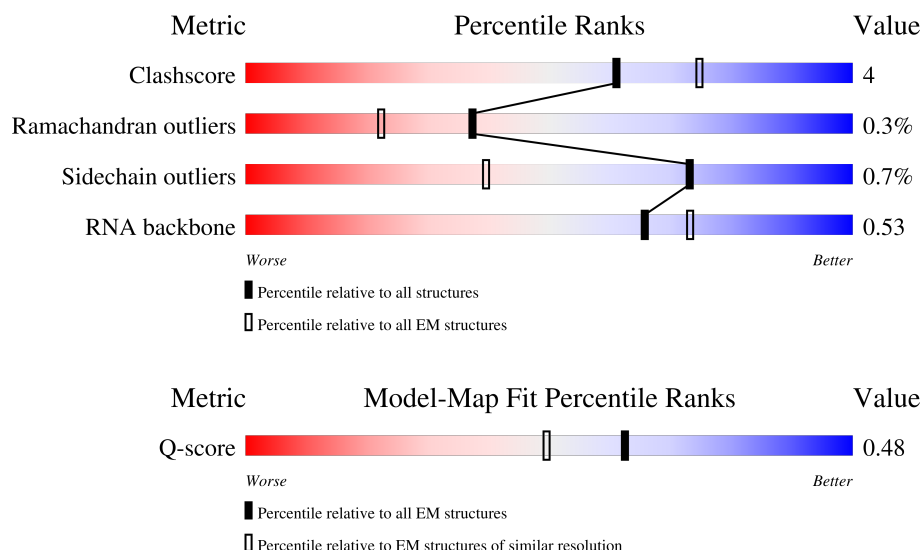
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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

Mol	Chain	Length	Quality of chain
1	2	3	
2	A	2883	
3	B	120	

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Mol	Chain	Length	Quality of chain
4	C	273	
5	D	209	
6	E	201	
7	F	179	
8	G	177	
9	H	149	
10	I	165	
11	J	142	
12	K	142	
13	L	123	
14	M	144	
15	N	136	
16	O	127	
17	P	117	
18	Q	115	
19	R	118	
20	S	103	
21	T	110	
22	U	100	
23	V	104	
24	W	94	
25	X	85	
26	Y	78	
27	Z	63	
28	a	59	

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Mol	Chain	Length	Quality of chain
29	b	57	84%14%
30	c	55	75%64%29%7%
31	d	46	87%13%
32	e	65	80%15%
33	f	38	87%13%
34	h	838	61%74%24%
35	k	57	53%86%14%

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 98708 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 tRNA-CCA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	2883	Total	C	N	O	P	0	0
			61902	27613	11397	20009	2883		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	272	Total	C	N	O	S	0	1
			2083	1288	424	364	7		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	178	Total	C	N	O	S	0	1
			1411	899	250	256	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 9 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 10 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	125	Total	C	N	O	S	0	0
			946	598	169	175	4		

- Molecule 11 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	134	Total	C	N	O	S	0	0
			979	619	169	185	6		

- Molecule 12 is a protein called 50S ribosomal protein L13.

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

- Molecule 13 is a protein called 50S ribosomal protein L14.

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

- Molecule 14 is a protein called 50S ribosomal protein L15.

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

- Molecule 15 is a protein called 50S ribosomal protein L16.

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

- Molecule 16 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	125	Total	C	N	O	S	0	0
			993	613	202	173	5		

- Molecule 17 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 18 is a protein called 50S ribosomal protein L19.

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

- Molecule 19 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	117	Total	C	N	O	S	0	0
			947	604	192	151			

- Molecule 20 is a protein called 50S ribosomal protein L21.

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

- Molecule 21 is a protein called 50S ribosomal protein L22.

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

- Molecule 22 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	92	Total	C	N	O	S	0	0
			730	461	138	130	1		

- Molecule 23 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	103	Total	C	N	O		0	1
			780	492	147	141			

- Molecule 24 is a protein called 50S ribosomal protein L25.

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

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	76	Total	C	N	O	S	0	0
			580	359	117	103	1		

- Molecule 26 is a protein called 50S ribosomal protein L28.

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

- Molecule 27 is a protein called 50S ribosomal protein L29.

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

- Molecule 28 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 29 is a protein called 50S ribosomal protein L32.

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

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	51	Total	C	N	O	S	0	0
			414	266	76	72			

- Molecule 31 is a protein called 50S ribosomal protein L34.

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

- Molecule 32 is a protein called 50S ribosomal protein L35.

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

- Molecule 33 is a protein called 50S ribosomal protein L36.

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

- Molecule 34 is a protein called Protein translocase subunit SecA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	838	Total	C	N	O	S	0	0
			6672	4181	1181	1276	34		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	-3	GLN	-	expression tag	UNP A0A037YQ84
h	-2	GLY	-	expression tag	UNP A0A037YQ84
h	-1	HIS	-	expression tag	UNP A0A037YQ84
h	0	MET	-	expression tag	UNP A0A037YQ84
h	12	CYS	SER	conflict	UNP A0A037YQ84

- Molecule 35 is a protein called Cytoskeleton protein RodZ.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	k	57	Total	C	N	O	S	0	0
			374	247	63	63	1		

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	A	65	Total	Mg	0
			65	65	
36	B	2	Total	Mg	0
			2	2	
36	b	1	Total	Mg	0
			1	1	

- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
37	f	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.

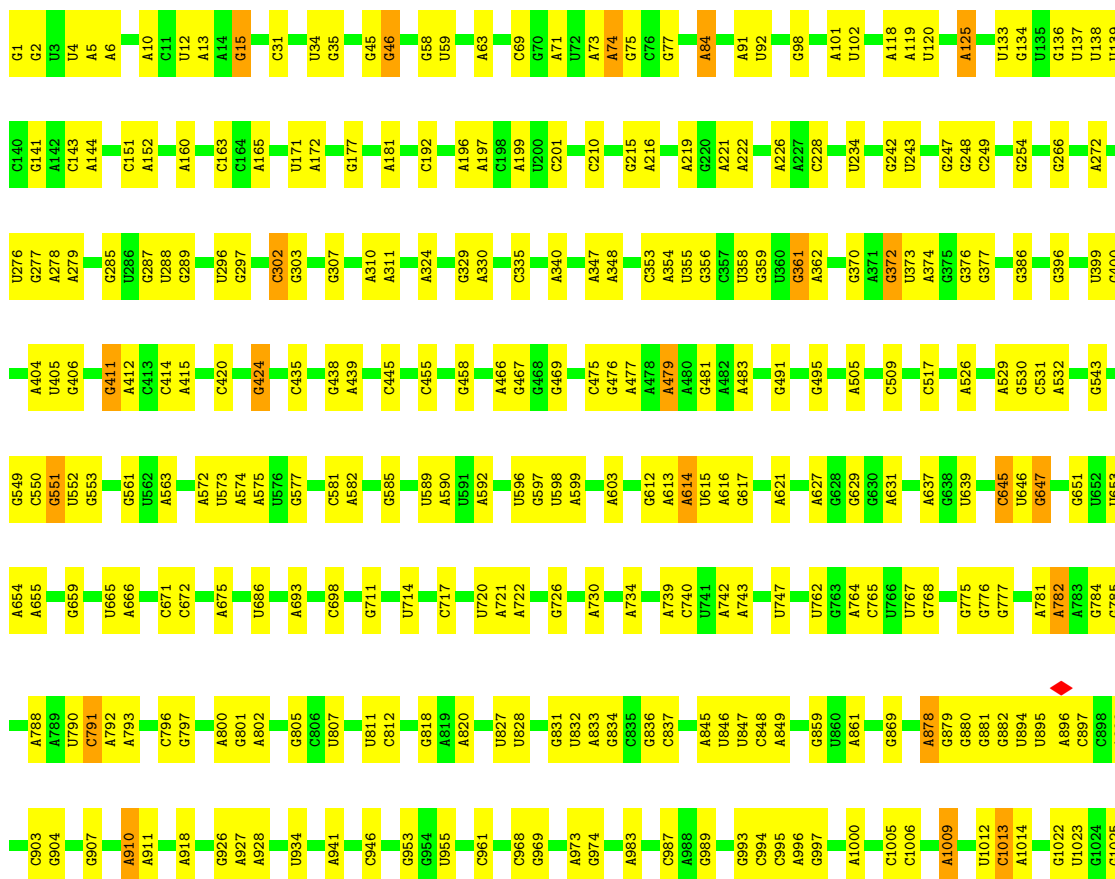
• Molecule 1: tRNA-CCA

Chain 2:  67% 33%

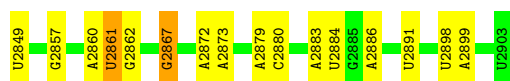


• Molecule 2: 23S ribosomal RNA

Chain A:  70% 27%



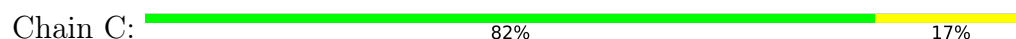
G1026	A1027	A1028	A1029	U1033	A1040	C1045	A1046	G1047	G1051	C1052	C1053	G1056	A1057	U1060	G1063	U1066	A1067	G1068	A1069	A1070	G1071	C1072	A1073	G1074	C1075	C1076	A1077	A1080	U1081	U1082	U1083	A1084	G1087	A1088	A1089	A1095	A1096	U1097	U1101	C1102	A1103	C1104	U1105	G1106	G1107	U1108									
G1112	U1113	C1114	G1115	G1122	C1123	G1124	G1128	U1132	A1133	C1135	U1141	A1142	C1153	G1154	A1155	G1168	A1169	U1173	G1177	C1178	G1179	U1180	U1181	G1182	U1188	A1205	G1212	G1218	G1227	G1236	A1237	G1238	A1244	A1247	G1250	A1253	A1254	U1255	G1256	U1263															
G1266	G1271	A1272	A1275	C1278	G1279	G1288	C1295	G1300	A1301	G1311	U1316	G1317	A1321	U1329	U1340	C1345	U1352	A1353	G1358	A1359	G1360	G1361	C1362	C1363	A1364	A1365	A1373	A1378	U1379	G1380	A1383	A1384	A1385	C1386	A1387	A1392	A1393	U1394	U1396																
G1408	G1416	C1417	G1421	A1427	C1428	G1429	G1430	G1432	A1433	A1434	G1435	A1436	C1437	G1447	G1448	G1451	G1452	A1453	U1457	U1460	A1469	A1470	A1477	G1482	G1491	G1492	A1493	A1494	A1495	U1497	A1508	A1509	G1510	G1511	G1514	A1515	G1524	A1528	G1529	C1533															
U1534	A1535	C1536	G1537	U1539	G1540	C1541	U1542	G1543	C1557	C1558	U1563	A1564	C1565	A1566	A1569	A1570	A1571	A1572	U1578	A1583	U1584	C1585	A1590	A1591	C1592	A1593	U1594	U1602	A1603	C1604	C1607	A1608	A1609	A1610	G1622	A1634	A1635	U1636	A1637	G1645	C1646	U1647	U1648	G1649	G1659										
G1667	A1668	A1669	C1670	U1671	A1672	G1673	G1674	G1681	G1682	U1688	A1698	G1699	A1700	G1710	A1711	G1715	G1724	U1729	C1730	G1731	C1732	G1733	G1734	A1735	U1736	G1737	G1738	G1743	A1744	A1745	G1756	A1757	U1758	A1759	A1762	G1763	C1764	A1773	U1779	A1780	U1781	U1782	A1783	A1784	G1797	U1798									
G1799	C1800	A1801	A1802	A1808	A1809	A1810	A1811	C1816	G1826	U1827	G1828	A1829	A1853	G1869	C1870	A1871	A1872	G1873	G1888	G1906	C1929	A1936	A1937	A1938	U1939	U1955	G1964	C1967	U1970	U1971	G1972	G1980	A1981	U1982	U1991	G1992	U1993	C1997	A1998	C1999	G2012														
A2020	C2023	A2030	A2031	A2032	A2033	A2034	U2039	G2040	C2043	C2047	G2048	C2055	G2056	A2060	G2061	A2062	G2069	A2070	A2071	U2076	U2079	A2080	A2082	U2086	G2087	A2088	G2093	A2097	U2098	U2099	G2100	C2104	U2105	U2106	G2107	A2108	U2109	G2110	U2111	U2112	U2113	A2114	G2115	G2116											
A2117	U2118	A2119	G2120	G2121	U2122	G2123	G2124	G2125	A2126	G2127	G2128	C2129	U2130	U2131	U2132	G2133	A2134	A2135	G2136	U2137	G2138	U2139	G2140	G2141	C2145	A2146	A2147	G2148	G2156	G2157	A2158	G2159	G2160	C2161	A2162	A2163	C2164	C2165	U2166	G2167	G2168	A2169	A2170	A2171	U2172	A2173	A2176	C2177	C2178	C2179	U2180	U2181	A2184	U2185	G2186
U2187	U2188	U2189	G2190	A2191	U2192	A2198	A2199	U2203	G2204	C2208	G2209	U2210	A2211	C2215	G2223	G2224	A2225	U2229	G2230	G2238	G2239	U2240	A2241	G2242	G2246	A2247	C2258	A2266	A2278	G2279	G2282	C2283	A2284	C2285	G2286	A2287	A2288	U2291	U2305	G2308	A2309	C2310	G2316												
A2317	A2322	G2325	A2328	U2329	A2333	U2334	A2335	C2339	A2340	C2347	U2348	G2349	C2350	G2361	C2374	G2383	U2384	C2385	U2390	G2391	U2402	G2405	A2406	A2407	A2411	G2415	U2419	C2422	U2423	C2424	A2425	A2426	C2427	G2428	G2429	A2430	U2431	A2432	A2433	A2434	A2435	U2441													
C2442	C2443	G2447	A2448	G2455	C2465	C2466	C2467	A2468	A2469	G2470	U2473	A2476	U2477	A2478	G2481	A2482	C2483	G2484	G2485	C2486	U2491	G2494	C2498	G2502	A2503	U2504	G2505	G2508	U2514	C2515	A2516	C2517	A2518	U2519	C2520	G2529	G2532	C2540	A2547	U2554	U2562														
A2566	G2567	A2572	G2581	U2584	C2585	U2586	C2591	G2592	U2595	A2598	G2602	G2603	U2609	U2613	A2614	U2615	G2621	G2627	A2628	U2629	C2636	C2646	U2647	G2648	A2654	G2655	U2656	G2663	G2664	A2665	C2681	A2682	C2683	U2684	U2687	G2688	U2689	U2690	U2698	C2699															
G2714	C2715	C2716	G2717	G2718	G2719	U2720	A2726	G2732	A2733	U2739	A2740	G2744	A2748	U2756	A2757	A2765	C2771	C2772	G2777	A2778	U2779	G2780	A2781	C2787	C2788	G2791	A2792	U2798	G2799	A2800	U2809	U2818	G2819	A2820	G2825	U2833	G2834	A2835	U2836	U2847	G2848														



- Molecule 3: 5S ribosomal RNA



- Molecule 4: 50S ribosomal protein L2



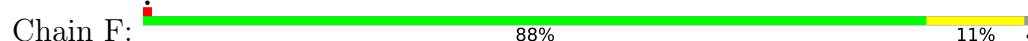
- Molecule 5: 50S ribosomal protein L3



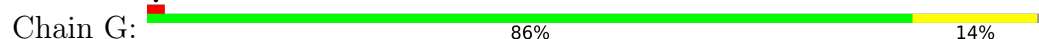
- Molecule 6: 50S ribosomal protein L4



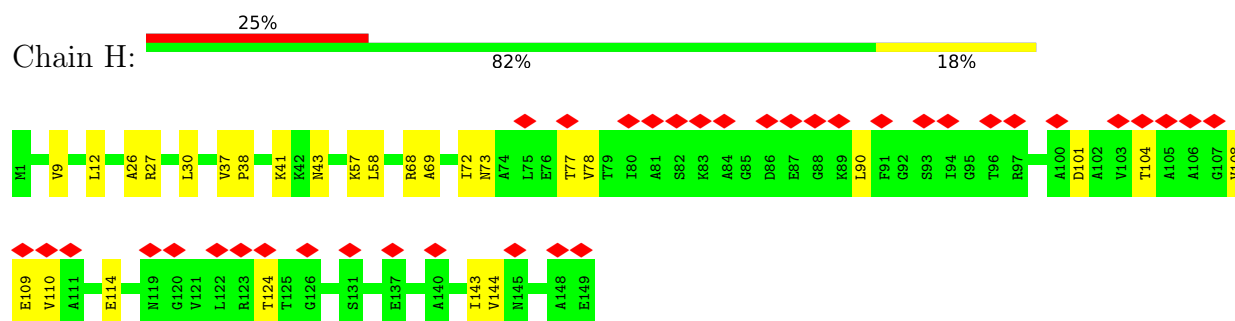
- Molecule 7: 50S ribosomal protein L5



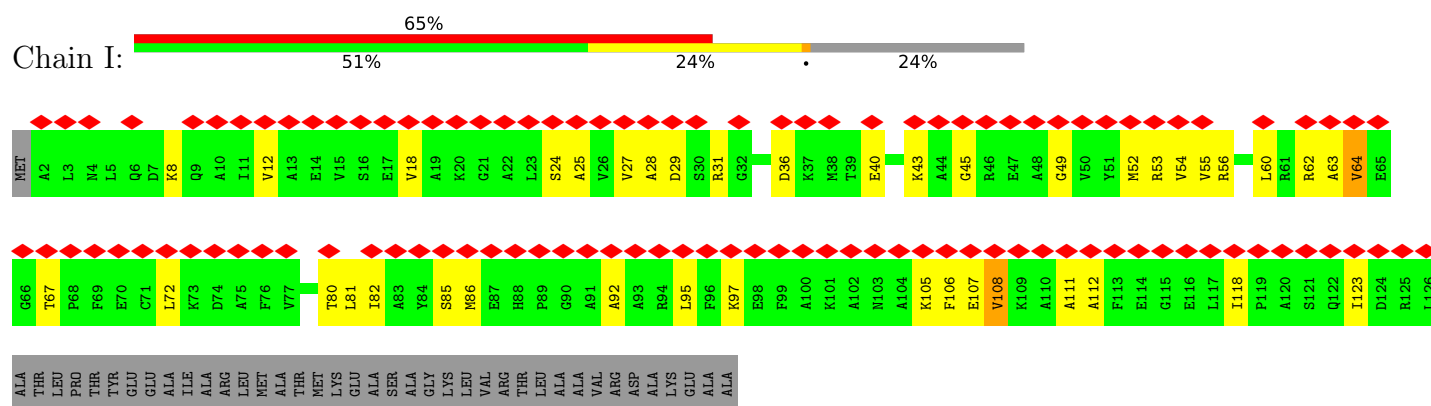
- Molecule 8: 50S ribosomal protein L6



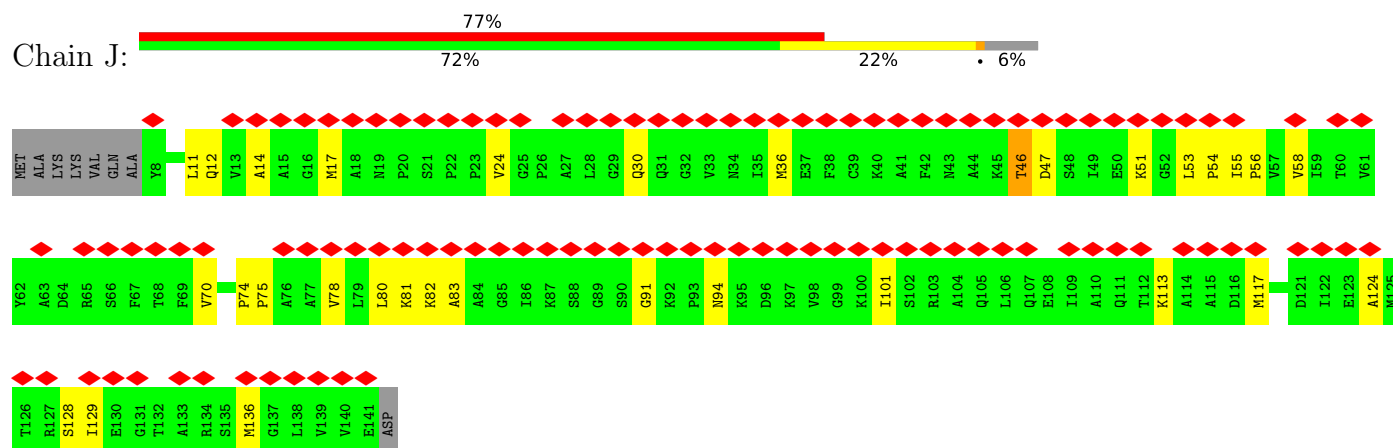
- Molecule 9: 50S ribosomal protein L9



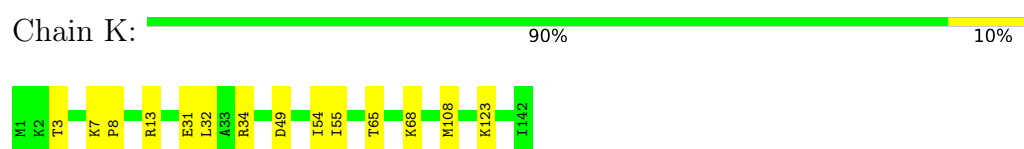
- Molecule 10: 50S ribosomal protein L10



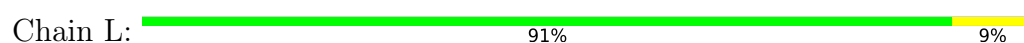
- Molecule 11: 50S ribosomal protein L11

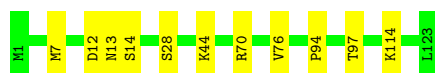


- Molecule 12: 50S ribosomal protein L13

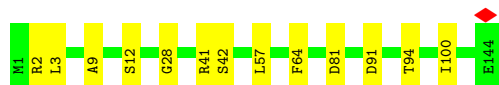


- Molecule 13: 50S ribosomal protein L14

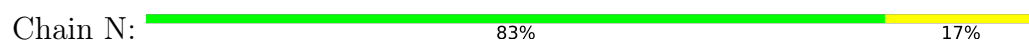




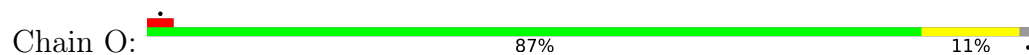
- Molecule 14: 50S ribosomal protein L15



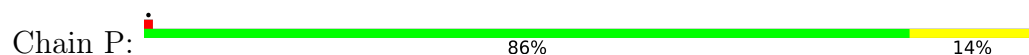
- Molecule 15: 50S ribosomal protein L16



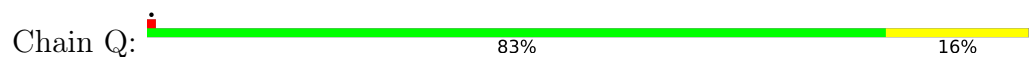
- Molecule 16: 50S ribosomal protein L17



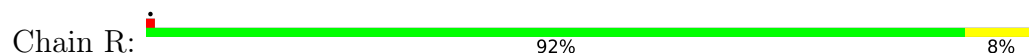
- Molecule 17: 50S ribosomal protein L18



- Molecule 18: 50S ribosomal protein L19



- Molecule 19: 50S ribosomal protein L20

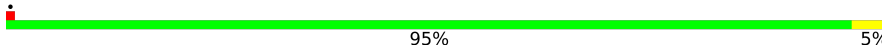


- Molecule 20: 50S ribosomal protein L21

Chain S:  90% 10%



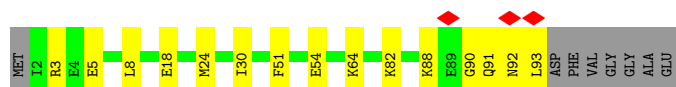
- Molecule 21: 50S ribosomal protein L22

Chain T:  95% 5%



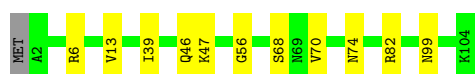
- Molecule 22: 50S ribosomal protein L23

Chain U:  77% 15% 8%



- Molecule 23: 50S ribosomal protein L24

Chain V:  88% 11%



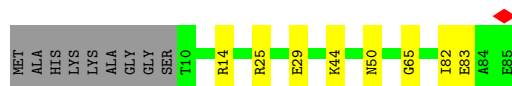
- Molecule 24: 50S ribosomal protein L25

Chain W:  86% 14%



- Molecule 25: 50S ribosomal protein L27

Chain X:  80% 9% 11%

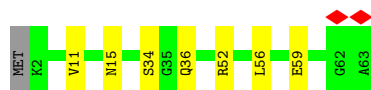
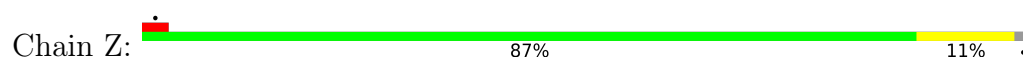


- Molecule 26: 50S ribosomal protein L28

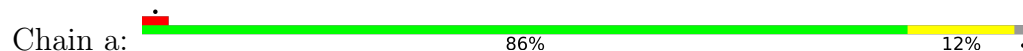
Chain Y:  81% 18%



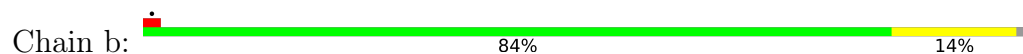
- Molecule 27: 50S ribosomal protein L29



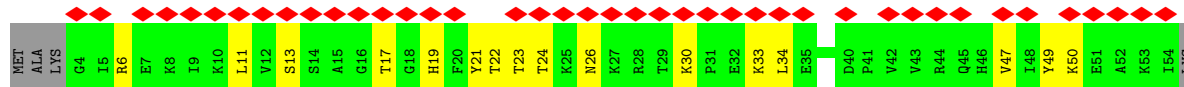
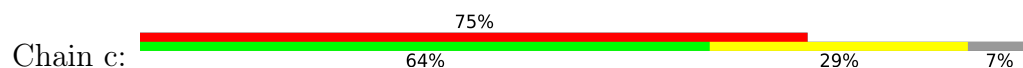
- Molecule 28: 50S ribosomal protein L30



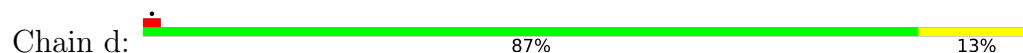
- Molecule 29: 50S ribosomal protein L32



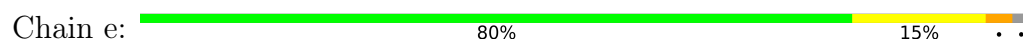
- Molecule 30: 50S ribosomal protein L33



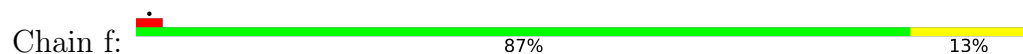
- Molecule 31: 50S ribosomal protein L34



- Molecule 32: 50S ribosomal protein L35

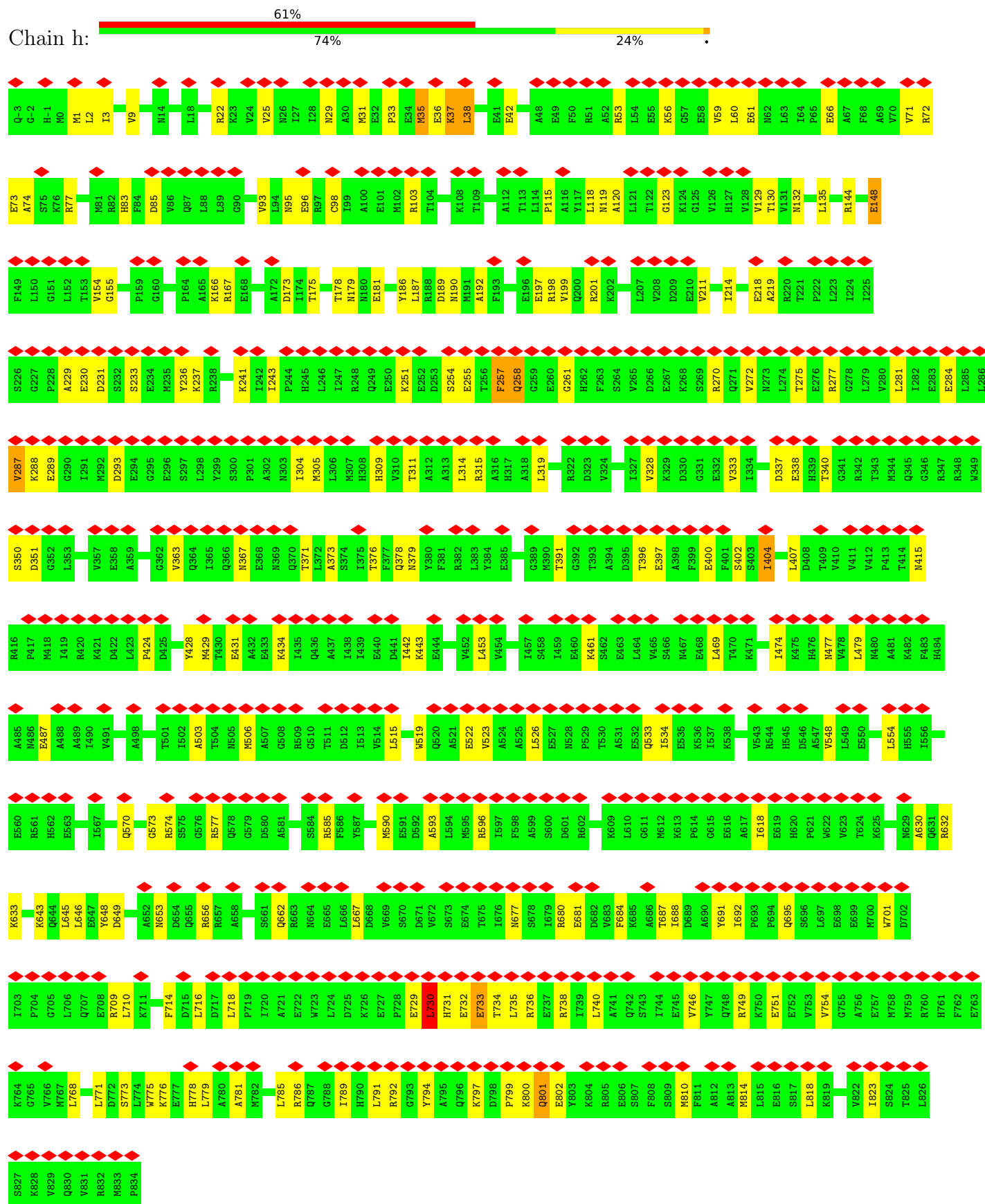


- Molecule 33: 50S ribosomal protein L36

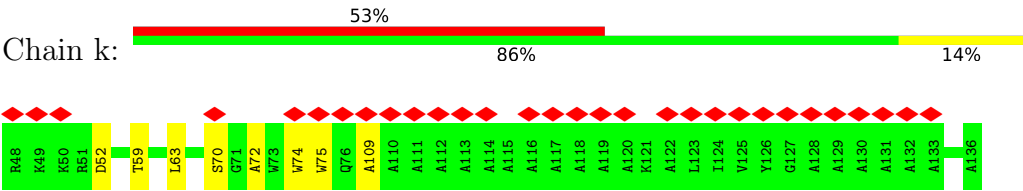


• Molecule 34: Protein translocase subunit SecA

Chain h:



● Molecule 35: Cytoskeleton protein RodZ



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	37334	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	6.126	Depositor
Minimum map value	-2.568	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.411	Depositor
Recommended contour level	0.82	Depositor
Map size ($\text{\AA}$)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.39, 1.39, 1.39	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	2	0.20	0/68	0.49	0/103
2	A	0.28	0/69329	0.36	0/108152
3	B	0.24	0/2872	0.33	0/4478
4	C	0.28	0/2122	0.49	0/2854
5	D	0.28	0/1586	0.45	0/2134
6	E	0.24	0/1571	0.42	0/2113
7	F	0.20	0/1435	0.47	0/1928
8	G	0.20	0/1343	0.44	0/1816
9	H	0.20	0/1121	0.53	2/1515 (0.1%)
10	I	0.30	0/958	0.69	0/1290
11	J	0.26	0/993	0.58	0/1341
12	K	0.26	0/1152	0.41	0/1551
13	L	0.27	0/955	0.45	0/1279
14	M	0.26	0/1062	0.45	0/1413
15	N	0.26	0/1093	0.45	0/1460
16	O	0.28	0/1006	0.54	0/1345
17	P	0.23	0/910	0.45	0/1219
18	Q	0.26	0/929	0.43	0/1242
19	R	0.25	0/960	0.41	0/1278
20	S	0.27	0/829	0.48	0/1107
21	T	0.27	0/864	0.47	0/1156
22	U	0.27	0/736	0.52	0/984
23	V	0.24	0/788	0.48	0/1053
24	W	0.23	0/766	0.46	0/1025
25	X	0.26	0/587	0.43	0/776
26	Y	0.29	0/635	0.50	0/848
27	Z	0.29	0/502	0.54	0/667
28	a	0.26	0/453	0.38	0/605
29	b	0.25	0/450	0.44	0/599
30	c	0.20	0/421	0.48	0/561
31	d	0.28	0/380	0.52	0/498
32	e	0.30	0/513	0.70	2/676 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	f	0.28	0/303	0.43	0/397
34	h	0.29	1/6782 (0.0%)	0.66	13/9146 (0.1%)
35	k	0.17	0/384	0.51	0/531
All	All	0.27	1/106858 (0.0%)	0.42	17/159140 (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
10	I	0	2
32	e	0	1
34	h	0	3
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	h	243	ILE	C-N	6.77	1.39	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	h	730	LEU	N-CA-C	7.79	119.86	111.36
34	h	733	GLU	CA-C-N	7.36	135.60	121.54
34	h	733	GLU	C-N-CA	7.36	135.60	121.54
34	h	800	LYS	CA-C-N	7.01	134.93	121.54
34	h	800	LYS	C-N-CA	7.01	134.93	121.54
32	e	32	ILE	N-CA-C	6.57	123.00	109.34
34	h	288	LYS	CA-C-N	6.37	136.85	126.86
34	h	288	LYS	C-N-CA	6.37	136.85	126.86
34	h	729	GLU	CA-C-N	5.91	128.69	120.29
34	h	729	GLU	C-N-CA	5.91	128.69	120.29
34	h	229	ALA	CA-C-N	5.85	132.72	121.54
34	h	229	ALA	C-N-CA	5.85	132.72	121.54
34	h	255	GLU	CA-C-N	5.76	132.55	121.54
34	h	255	GLU	C-N-CA	5.76	132.55	121.54
32	e	33	LEU	N-CA-C	5.16	121.80	110.80
9	H	37	VAL	CB-CA-C	5.04	114.27	109.33
9	H	37	VAL	N-CA-C	-5.03	105.07	109.19

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	I	105	LYS	Peptide
10	I	107	GLU	Peptide
32	e	31	HIS	Peptide
34	h	289	GLU	Peptide
34	h	618	ILE	Peptide
34	h	801	GLN	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	2	62	0	34	0	0
2	A	61902	0	31132	337	0
3	B	2569	0	1301	15	0
4	C	2083	0	2154	30	0
5	D	1565	0	1616	12	0
6	E	1552	0	1619	11	0
7	F	1411	0	1444	13	0
8	G	1323	0	1371	13	0
9	H	1110	0	1148	16	0
10	I	946	0	976	24	0
11	J	979	0	1028	21	0
12	K	1129	0	1162	9	0
13	L	946	0	1023	6	0
14	M	1053	0	1129	10	0
15	N	1074	0	1157	16	0
16	O	993	0	1034	7	0
17	P	900	0	935	11	0
18	Q	917	0	962	12	0
19	R	947	0	1019	8	0
20	S	816	0	839	7	0
21	T	857	0	922	3	0
22	U	730	0	795	11	0
23	V	780	0	831	9	0
24	W	753	0	780	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	X	580	0	594	5	0
26	Y	625	0	652	11	0
27	Z	501	0	531	5	0
28	a	449	0	488	3	0
29	b	444	0	458	6	0
30	c	414	0	442	13	0
31	d	377	0	418	5	0
32	e	504	0	572	9	0
33	f	302	0	340	5	0
34	h	6672	0	6667	133	0
35	k	374	0	333	9	0
36	A	65	0	0	0	0
36	B	2	0	0	0	0
36	b	1	0	0	0	0
37	f	1	0	0	0	0
All	All	98708	0	67906	706	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 (706) 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)
34:h:37:LYS:HB3	34:h:42:GLU:OE1	1.63	0.96
2:A:2100:G:H1	2:A:2189:U:H3	1.12	0.91
2:A:285:G:H1	2:A:355:U:H3	1.19	0.91
2:A:881:G:H1	2:A:895:U:H3	1.17	0.90
34:h:35:MET:HG3	34:h:73:GLU:HG2	1.55	0.88
2:A:711:G:H1	2:A:720:U:H3	1.25	0.83
34:h:38:LEU:HA	34:h:77:ARG:HD2	1.62	0.81
34:h:144:ARG:O	34:h:148:GLU:HB2	1.81	0.79
10:I:18:VAL:HG23	10:I:86:MET:CE	2.20	0.71
34:h:37:LYS:CB	34:h:42:GLU:OE1	2.39	0.70
9:H:69:ALA:O	9:H:73:ASN:HB2	1.93	0.67
34:h:799:PRO:HA	34:h:802:GLU:HB3	1.78	0.66
34:h:72:ARG:HG3	34:h:83:HIS:HB2	1.78	0.66
2:A:475:C:O2	2:A:479:A:N6	2.28	0.65
34:h:9:VAL:HG22	35:k:52:ASP:HB3	1.77	0.65
2:A:1408:G:H1	2:A:1594:U:H3	1.43	0.64
16:O:77:ALA:O	16:O:81:ASN:HB2	1.99	0.64
2:A:1607:C:N4	2:A:1622:G:OP2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:88:LYS:HG2	17:P:116:GLN:HG3	1.81	0.62
34:h:730:LEU:H	34:h:730:LEU:CD2	2.12	0.62
17:P:31:THR:HG22	17:P:33:ARG:H	1.65	0.62
34:h:85:ASP:HB2	34:h:415:ASN:HD21	1.64	0.62
2:A:77:G:OP1	27:Z:52:ARG:NH2	2.34	0.61
2:A:882:G:H1	2:A:894:U:H3	1.45	0.61
2:A:197:A:N6	2:A:2431:U:O2	2.33	0.61
8:G:99:LYS:HZ2	8:G:104:ASN:HB2	1.64	0.61
34:h:179:ASN:HD22	34:h:214:ILE:HD12	1.65	0.61
5:D:13:ARG:HH12	18:Q:75:GLN:HE21	1.48	0.61
10:I:18:VAL:HG23	10:I:86:MET:HE2	1.84	0.60
2:A:1102:C:H2'	2:A:1103:A:H8	1.66	0.60
2:A:2122:U:H3	2:A:2176:A:H61	1.48	0.60
34:h:251:LYS:HB3	34:h:284:GLU:HG3	1.84	0.60
3:B:43:C:O2	7:F:92:ARG:NH2	2.35	0.59
10:I:25:ALA:HB3	10:I:112:ALA:HB3	1.82	0.59
2:A:1528:A:N6	2:A:1543:G:O2'	2.35	0.59
2:A:466:A:OP1	31:d:34:ARG:NH1	2.35	0.59
2:A:495:G:N3	21:T:61:ASN:ND2	2.50	0.59
9:H:38:PRO:O	9:H:43:ASN:ND2	2.35	0.59
2:A:1529:G:H1	2:A:1542:U:H3	1.51	0.59
2:A:2771:C:O2'	5:D:173:GLN:NE2	2.34	0.59
2:A:2286:G:H5'	30:c:30:LYS:HZ2	1.68	0.58
34:h:38:LEU:O	34:h:77:ARG:NH1	2.35	0.58
34:h:677:ASN:OD1	34:h:680:ARG:NH2	2.37	0.57
26:Y:59:ILE:HG12	26:Y:67:VAL:HG21	1.85	0.57
34:h:258:GLN:HB2	34:h:261:GLY:HA2	1.85	0.57
34:h:103:ARG:HE	34:h:577:ARG:HA	1.70	0.57
2:A:574:A:N6	2:A:2034:U:OP1	2.38	0.57
2:A:2128:G:N3	2:A:2173:A:O2'	2.35	0.57
10:I:60:LEU:O	10:I:64:VAL:HB	2.04	0.57
34:h:523:VAL:HG11	34:h:534:ILE:HG23	1.87	0.57
2:A:1047:G:OP1	10:I:56:ARG:NH1	2.38	0.57
7:F:33:LYS:HG3	7:F:157:THR:HB	1.87	0.57
34:h:570:GLN:O	34:h:574:ARG:NH2	2.37	0.57
2:A:445:C:OP1	19:R:2:ALA:N	2.38	0.56
2:A:2131:U:H5'	2:A:2132:U:H5''	1.86	0.56
2:A:2848:G:O2'	2:A:2867:G:N2	2.35	0.56
4:C:84:ASP:OD1	4:C:86:ASN:ND2	2.38	0.56
11:J:78:VAL:HA	11:J:81:LYS:HD2	1.87	0.56
8:G:42:GLU:HA	8:G:55:ARG:HH21	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:614:A:O2'	2:A:616:A:N7	2.38	0.56
2:A:340:A:O2'	6:E:162:ARG:NH1	2.39	0.56
2:A:1070:A:N7	2:A:1096:A:O2'	2.38	0.56
2:A:1798:U:OP2	4:C:271:ARG:NH2	2.37	0.56
2:A:2508:G:HO2'	2:A:2554:U:HO2'	1.51	0.56
29:b:54:VAL:HG23	29:b:55:ILE:HG12	1.87	0.56
3:B:1:U:H2'	3:B:2:G:H8	1.71	0.56
8:G:22:GLN:NE2	8:G:38:ASN:O	2.38	0.56
22:U:93:LEU:HD22	35:k:59:THR:HG23	1.88	0.56
34:h:192:ALA:HB1	34:h:197:GLU:HB2	1.88	0.56
34:h:376:THR:HG21	34:h:649:ASP:HB3	1.87	0.56
8:G:16:ASP:HB3	8:G:27:LYS:HB2	1.88	0.56
2:A:1066:U:N3	2:A:1069:A:OP2	2.39	0.56
2:A:1808:A:O2'	26:Y:3:ARG:NH1	2.39	0.56
26:Y:43:GLU:OE2	26:Y:45:ARG:NH2	2.39	0.56
2:A:1081:U:H4'	11:J:124:ALA:HB1	1.89	0.55
34:h:29:ASN:HB3	34:h:72:ARG:HH22	1.71	0.55
34:h:38:LEU:O	34:h:77:ARG:CZ	2.54	0.55
34:h:115:PRO:O	34:h:119:ASN:ND2	2.37	0.55
2:A:1826:G:O2'	2:A:1971:U:OP2	2.25	0.55
16:O:28:LEU:HD23	16:O:48:VAL:HG21	1.89	0.55
17:P:34:HIS:ND1	17:P:53:THR:OG1	2.39	0.55
34:h:751:GLU:HA	34:h:754:VAL:HG12	1.88	0.55
2:A:1063:G:N2	11:J:91:GLY:O	2.39	0.55
2:A:2720:U:OP1	18:Q:53:ARG:NH2	2.40	0.55
20:S:65:ALA:HB3	20:S:95:ASP:HB2	1.88	0.55
34:h:810:MET:HE3	34:h:814:MET:HB2	1.88	0.55
2:A:2114:A:N6	2:A:2167:U:O2'	2.39	0.55
10:I:24:SER:HB2	10:I:85:SER:HB3	1.88	0.55
34:h:120:ALA:HB1	34:h:173:ASP:HB3	1.89	0.55
34:h:219:ALA:O	34:h:376:THR:OG1	2.25	0.55
11:J:17:MET:SD	11:J:51:LYS:NZ	2.74	0.55
8:G:170:ARG:NH2	33:f:29:ALA:O	2.39	0.54
2:A:617:G:OP1	6:E:102:ARG:NH2	2.40	0.54
2:A:1539:U:H2'	2:A:1540:G:H8	1.73	0.54
9:H:27:ARG:NH2	26:Y:60:ASP:OD2	2.40	0.54
2:A:781:A:OP1	4:C:217:ARG:NH2	2.40	0.54
4:C:132:MET:HG2	4:C:135:ILE:HD12	1.89	0.54
11:J:56:PRO:HD3	11:J:75:PRO:HG3	1.88	0.54
2:A:807:U:OP2	14:M:41:ARG:NH1	2.40	0.54
2:A:612:G:N2	2:A:614:A:O2'	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1528:A:OP2	2:A:1543:G:N2	2.38	0.54
2:A:1724:G:O6	2:A:1737:G:N2	2.41	0.54
11:J:46:THR:HG21	11:J:55:ILE:HG21	1.90	0.54
34:h:25:VAL:HG13	34:h:29:ASN:HD21	1.73	0.53
34:h:371:THR:HG22	34:h:779:LEU:HD13	1.89	0.53
34:h:429:MET:HA	34:h:590:MET:HG3	1.89	0.53
2:A:994:C:O2	20:S:10:LYS:NZ	2.41	0.53
2:A:2079:U:O2'	26:Y:23:ASN:OD1	2.27	0.53
9:H:68:ARG:NH2	9:H:114:GLU:OE2	2.41	0.53
2:A:1046:A:H5'	10:I:62:ARG:HE	1.72	0.53
2:A:210:C:OP1	31:d:29:GLN:NE2	2.36	0.53
2:A:92:U:O2	35:k:109:ALA:N	2.41	0.53
2:A:411:G:OP2	2:A:2406:A:O2'	2.26	0.53
2:A:2566:A:N1	13:L:28:SER:OG	2.39	0.53
34:h:186:TYR:O	34:h:190:ASN:ND2	2.39	0.53
2:A:848:C:H2'	2:A:849:A:H8	1.74	0.53
7:F:29:PRO:HB2	7:F:169:LEU:HD22	1.91	0.53
2:A:1275:A:OP2	2:A:1646:C:N4	2.42	0.53
16:O:59:SER:OG	16:O:62:ASN:ND2	2.41	0.53
2:A:629:G:N3	2:A:639:U:O2'	2.42	0.53
10:I:29:ASP:HB3	10:I:106:PHE:HB2	1.89	0.53
13:L:7:MET:HE1	13:L:44:LYS:HG3	1.90	0.53
34:h:59:VAL:HG12	34:h:61:GLU:H	1.74	0.53
2:A:243:U:OP2	32:e:8:ARG:NH1	2.42	0.53
2:A:2581:G:N2	2:A:2581:G:OP2	2.42	0.53
5:D:39:ASP:N	5:D:39:ASP:OD1	2.42	0.53
2:A:278:A:OP2	2:A:361:G:N1	2.40	0.52
4:C:72:ASP:OD2	4:C:189:ARG:NH1	2.40	0.52
26:Y:72:ARG:NH2	26:Y:78:TYR:OH	2.41	0.52
2:A:125:A:OP2	31:d:19:ARG:NH2	2.40	0.52
34:h:515:LEU:HD21	34:h:554:LEU:HB2	1.91	0.52
4:C:144:VAL:HB	4:C:154:LEU:HB2	1.91	0.52
17:P:25:ARG:NH2	17:P:93:ASP:OD2	2.42	0.52
2:A:1009:A:N3	2:A:1153:C:O2'	2.40	0.52
34:h:237:LYS:O	34:h:241:LYS:HB2	2.09	0.52
34:h:773:SER:HA	34:h:776:LYS:HE3	1.90	0.52
2:A:13:A:O2'	2:A:15:G:N7	2.41	0.52
2:A:358:U:H2'	2:A:359:G:H8	1.73	0.52
8:G:101:ASN:ND2	8:G:116:GLN:OE1	2.43	0.52
2:A:955:U:OP1	15:N:86:LYS:NZ	2.41	0.52
2:A:987:C:O2'	2:A:1000:A:N3	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2282:G:N2	2:A:2390:U:O2	2.37	0.52
8:G:18:LYS:HB3	8:G:25:THR:HB	1.91	0.52
10:I:40:GLU:HA	10:I:43:LYS:HE3	1.91	0.52
2:A:2788:C:O2'	2:A:2809:A:N3	2.40	0.52
34:h:645:LEU:HD23	34:h:648:TYR:HD2	1.75	0.52
2:A:881:G:O6	2:A:895:U:O4	2.27	0.52
3:B:37:C:O2	17:P:100:HIS:NE2	2.41	0.52
7:F:36:LEU:HB3	7:F:152:LEU:HD21	1.91	0.52
34:h:688:ILE:HD13	34:h:736:ARG:HG2	1.91	0.52
34:h:730:LEU:CD2	34:h:730:LEU:N	2.73	0.52
6:E:184:ASP:OD1	14:M:2:ARG:NH2	2.43	0.51
2:A:1046:A:H1'	10:I:8:LYS:HD2	1.92	0.51
2:A:2469:A:N6	2:A:2481:G:O2'	2.43	0.51
6:E:119:ILE:HB	6:E:187:VAL:HG22	1.92	0.51
10:I:45:GLY:O	10:I:49:GLY:N	2.42	0.51
2:A:2258:C:O2'	2:A:2427:C:OP2	2.27	0.51
2:A:2473:U:O4	8:G:176:LYS:NZ	2.43	0.51
11:J:53:LEU:HD11	11:J:82:LYS:HG3	1.93	0.51
2:A:1057:A:O2'	10:I:36:ASP:OD1	2.28	0.51
2:A:1080:A:H1'	11:J:128:SER:HA	1.92	0.51
2:A:1392:A:N6	22:U:18:GLU:OE1	2.43	0.51
11:J:81:LYS:HG3	11:J:136:MET:HE1	1.92	0.51
34:h:236:TYR:OH	34:h:309:HIS:O	2.24	0.51
2:A:2286:G:OP2	30:c:6:ARG:NH2	2.44	0.51
2:A:2540:C:O2'	2:A:2740:A:N3	2.40	0.51
12:K:13:ARG:NH1	12:K:49:ASP:O	2.43	0.51
16:O:103:ARG:HH21	16:O:110:MET:HE1	1.76	0.51
34:h:337:ASP:OD2	34:h:340:THR:OG1	2.28	0.51
34:h:691:TYR:OH	34:h:709:ARG:NH1	2.44	0.51
2:A:254:G:N7	32:e:5:LYS:NZ	2.55	0.51
2:A:1386:C:H2'	2:A:1387:A:H8	1.75	0.51
34:h:214:ILE:HA	34:h:218:GLU:HB3	1.92	0.51
2:A:2405:G:O2'	2:A:2411:A:N6	2.40	0.51
10:I:53:ARG:HG2	10:I:55:VAL:HG13	1.94	0.50
14:M:91:ASP:H	14:M:94:THR:HB	1.76	0.50
34:h:716:LEU:HD23	34:h:718:LEU:HD21	1.93	0.50
2:A:1340:U:OP2	22:U:82:LYS:NZ	2.43	0.50
2:A:2291:U:O2'	2:A:2374:C:O2	2.29	0.50
2:A:2646:C:OP2	2:A:2732:G:O2'	2.29	0.50
34:h:424:PRO:O	34:h:585:ARG:NH2	2.45	0.50
2:A:561:G:HO2'	19:R:45:TYR:HH	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1051:G:H1	2:A:1108:U:H3	1.58	0.50
2:A:2424:C:H5'	2:A:2425:A:H5'	1.91	0.50
34:h:233:SER:HB2	34:h:367:ASN:HA	1.92	0.50
34:h:315:ARG:HA	34:h:319:LEU:HD23	1.93	0.50
34:h:506:MET:SD	34:h:574:ARG:NH1	2.79	0.50
4:C:66:ASP:OD2	4:C:102:ARG:NH1	2.42	0.50
34:h:251:LYS:H	34:h:281:LEU:HD22	1.76	0.50
2:A:1053:C:O2	10:I:31:ARG:NH2	2.41	0.50
33:f:8:LYS:O	33:f:35:GLN:NE2	2.45	0.50
2:A:1602:U:OP2	22:U:64:LYS:NZ	2.38	0.50
14:M:81:ASP:HB3	14:M:100:ILE:HD13	1.92	0.50
34:h:144:ARG:NH1	34:h:154:VAL:O	2.39	0.50
34:h:166:LYS:NZ	34:h:181:GLU:OE2	2.42	0.50
34:h:254:SER:HB3	34:h:257:PHE:HB2	1.94	0.50
2:A:1539:U:H2'	2:A:1540:G:C8	2.46	0.50
2:A:2171:A:O2'	2:A:2173:A:OP1	2.30	0.50
10:I:27:VAL:HG13	10:I:80:THR:HG23	1.92	0.50
32:e:24:HIS:ND1	32:e:25:LYS:O	2.44	0.50
34:h:95:ASN:ND2	34:h:96:GLU:OE2	2.45	0.50
34:h:710:LEU:O	34:h:714:PHE:HB2	2.11	0.50
2:A:249:C:O2	32:e:12:LYS:NZ	2.42	0.50
2:A:577:G:O2'	2:A:1254:A:OP1	2.30	0.50
2:A:878:A:H3'	2:A:879:G:H8	1.76	0.50
2:A:1022:G:O6	12:K:68:LYS:NZ	2.45	0.50
4:C:8:PRO:HB3	4:C:14:ARG:HG3	1.94	0.50
7:F:102:ARG:NH2	7:F:140:GLU:OE2	2.45	0.50
34:h:593:ALA:HA	34:h:596:ARG:HG2	1.93	0.50
2:A:1358:G:O2'	2:A:1373:A:N6	2.45	0.49
2:A:1671:U:O2'	2:A:1673:G:N7	2.43	0.49
4:C:166:ALA:HB3	4:C:173:THR:HB	1.92	0.49
28:a:40:ASP:OD2	28:a:45:ARG:NH1	2.41	0.49
34:h:53:ARG:HA	34:h:56:LYS:HE2	1.94	0.49
34:h:376:THR:HG23	34:h:379:ASN:HB2	1.93	0.49
2:A:335:C:O2	23:V:68:SER:OG	2.28	0.49
2:A:672:C:OP2	14:M:42:SER:OG	2.27	0.49
2:A:2431:U:H5	2:A:2433:A:H5''	1.77	0.49
34:h:53:ARG:NH2	34:h:66:GLU:OE1	2.42	0.49
2:A:335:C:OP2	23:V:82:ARG:NH2	2.45	0.49
2:A:1797:G:HO2'	4:C:257:THR:HG1	1.59	0.49
2:A:1006:C:O2'	12:K:108:MET:O	2.29	0.49
2:A:1869:G:N2	2:A:1871:A:O2'	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2502:G:H5''	2:A:2503:A:H5''	1.93	0.49
34:h:746:VAL:HG22	34:h:749:ARG:HH12	1.77	0.49
2:A:307:G:N1	2:A:310:A:OP2	2.39	0.49
2:A:2349:G:OP1	32:e:45:ARG:NH2	2.44	0.49
2:A:2636:C:O2'	5:D:45:TYR:OH	2.30	0.49
34:h:402:SER:HA	34:h:407:LEU:H	1.78	0.49
2:A:693:A:O2'	2:A:1353:A:N3	2.39	0.49
2:A:878:A:N6	2:A:899:A:O2'	2.45	0.49
2:A:1068:G:N2	2:A:1095:A:O3'	2.46	0.49
22:U:90:GLY:O	22:U:92:ASN:ND2	2.45	0.49
34:h:275:THR:HB	34:h:277:ARG:HG2	1.94	0.49
34:h:526:LEU:HD13	34:h:533:GLN:HE21	1.77	0.49
2:A:585:G:N7	19:R:6:ARG:NH1	2.61	0.49
2:A:1386:C:H2'	2:A:1387:A:C8	2.46	0.49
17:P:28:VAL:HG11	17:P:103:VAL:HG13	1.94	0.49
24:W:51:GLN:OE1	24:W:57:TYR:OH	2.30	0.49
34:h:350:SER:OG	34:h:351:ASP:N	2.45	0.49
4:C:152:GLY:O	4:C:156:ARG:NH2	2.44	0.49
17:P:27:VAL:HA	17:P:93:ASP:HB3	1.94	0.48
34:h:730:LEU:N	34:h:730:LEU:HD23	2.28	0.48
20:S:34:GLU:OE2	20:S:60:LYS:NZ	2.46	0.48
34:h:469:LEU:HD13	34:h:474:ILE:HD11	1.95	0.48
34:h:648:TYR:HB3	34:h:786:ARG:HH21	1.78	0.48
2:A:807:U:O2'	2:A:2060:A:N1	2.46	0.48
2:A:1797:G:O2'	4:C:257:THR:OG1	2.30	0.48
34:h:662:GLN:HE22	34:h:771:LEU:HD11	1.77	0.48
2:A:201:C:OP1	26:Y:18:ARG:NH1	2.46	0.48
2:A:1266:G:O2'	2:A:2012:G:O6	2.29	0.48
4:C:227:PRO:HG3	4:C:234:GLY:H	1.79	0.48
27:Z:11:VAL:O	27:Z:15:ASN:ND2	2.45	0.48
34:h:167:ARG:HG2	34:h:199:VAL:HA	1.96	0.48
34:h:431:GLU:OE1	34:h:434:LYS:NZ	2.45	0.48
34:h:653:ASN:HA	34:h:656:ARG:HB2	1.95	0.48
2:A:2229:U:H2'	2:A:2230:G:H8	1.79	0.48
15:N:66:ARG:NH1	15:N:104:GLU:OE1	2.39	0.48
18:Q:26:VAL:O	18:Q:44:GLU:HA	2.12	0.48
34:h:270:ARG:NH2	34:h:338:GLU:OE1	2.46	0.48
2:A:2515:C:H2'	2:A:2516:A:H8	1.79	0.48
2:A:2595:G:N2	2:A:2598:A:OP2	2.41	0.48
6:E:168:ASP:OD2	6:E:170:ARG:NH1	2.44	0.48
10:I:25:ALA:HB1	10:I:82:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:84:A:H5''	23:V:6:ARG:HG2	1.96	0.48
2:A:788:A:OP1	2:A:791:C:N4	2.37	0.48
2:A:1682:G:OP2	2:A:1699:G:N2	2.41	0.48
27:Z:36:GLN:NE2	35:k:70:SER:O	2.44	0.48
34:h:371:THR:HB	34:h:779:LEU:HB3	1.96	0.48
2:A:370:G:O2'	2:A:424:G:OP1	2.27	0.48
2:A:820:A:H4'	2:A:836:G:H22	1.78	0.48
2:A:2305:U:H5''	7:F:131:GLY:HA3	1.95	0.48
34:h:684:PHE:HA	34:h:687:THR:HG22	1.96	0.48
2:A:1800:C:H5'	4:C:146:MET:HE1	1.95	0.48
2:A:2246:G:H2'	2:A:2247:A:H8	1.79	0.48
2:A:2483:C:N3	15:N:123:LYS:NZ	2.50	0.48
31:d:34:ARG:NH2	31:d:41:ARG:O	2.46	0.48
34:h:73:GLU:HB3	34:h:77:ARG:HE	1.79	0.48
34:h:328:VAL:HG22	34:h:333:VAL:HG12	1.95	0.48
2:A:45:G:H5''	2:A:46:G:H5'	1.96	0.48
2:A:517:C:OP1	29:b:13:ARG:NH2	2.44	0.48
4:C:5:LYS:NZ	4:C:14:ARG:O	2.47	0.48
4:C:100:GLU:OE2	4:C:102:ARG:NE	2.41	0.48
34:h:187:LEU:HD22	34:h:373:ALA:HB1	1.96	0.48
2:A:818:G:N1	2:A:1188:U:OP2	2.35	0.47
2:A:1105:U:H2'	2:A:1106:G:H8	1.79	0.47
2:A:1853:A:N6	2:A:1888:G:O2'	2.47	0.47
8:G:90:VAL:O	8:G:160:LYS:HA	2.14	0.47
19:R:49:ASP:HA	19:R:52:GLN:HB2	1.95	0.47
29:b:43:ILE:HG22	29:b:49:TYR:HB2	1.96	0.47
2:A:1999:C:O2	2:A:2687:U:O2'	2.32	0.47
34:h:735:LEU:HA	34:h:738:ARG:HD3	1.96	0.47
2:A:458:G:O2'	2:A:469:G:O6	2.29	0.47
2:A:918:A:N3	3:B:80:U:O2'	2.46	0.47
9:H:104:THR:HG22	9:H:109:GLU:HA	1.96	0.47
2:A:171:U:H2'	2:A:172:A:H8	1.79	0.47
2:A:1744:A:H3'	2:A:1745:A:H8	1.79	0.47
2:A:2047:C:H2'	2:A:2048:G:H8	1.78	0.47
34:h:453:LEU:HD11	34:h:503:ALA:HB2	1.96	0.47
34:h:778:HIS:HB2	34:h:814:MET:HG3	1.96	0.47
2:A:995:C:O2	12:K:3:THR:OG1	2.32	0.47
2:A:2116:G:O6	2:A:2171:A:N6	2.47	0.47
9:H:77:THR:HG23	9:H:143:ILE:HB	1.95	0.47
34:h:123:GLY:O	34:h:201:ARG:NH1	2.48	0.47
2:A:698:C:O2'	2:A:734:A:N6	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:e:51:SER:OG	32:e:52:LYS:N	2.47	0.47
34:h:681:GLU:HG2	34:h:740:LEU:HD21	1.97	0.47
2:A:1278:C:H2'	2:A:1279:G:H8	1.79	0.47
4:C:164:ILE:HG12	4:C:174:LEU:HD23	1.96	0.47
15:N:41:LEU:HG	15:N:96:ILE:HG13	1.95	0.47
24:W:30:ILE:HG12	24:W:91:PHE:HB2	1.97	0.47
34:h:397:GLU:HG3	35:k:74:TRP:HA	1.97	0.47
2:A:1013:C:H2'	2:A:1014:A:H8	1.80	0.47
2:A:1779:U:OP2	2:A:1784:A:N6	2.40	0.47
14:M:28:GLY:HA3	20:S:82:HIS:HE1	1.80	0.47
17:P:99:TYR:OH	17:P:111:ARG:NH1	2.46	0.47
2:A:228:C:N4	2:A:2407:A:N3	2.63	0.47
2:A:1168:G:H1	2:A:1181:U:H3	1.62	0.47
2:A:2246:G:H2'	2:A:2247:A:C8	2.50	0.47
11:J:83:ALA:HB3	11:J:101:ILE:HD12	1.97	0.47
34:h:31:MET:HE3	34:h:33:PRO:HG3	1.97	0.47
34:h:103:ARG:NH1	34:h:573:GLY:O	2.48	0.47
2:A:373:U:H2'	2:A:374:A:H8	1.80	0.46
2:A:1394:U:H4'	2:A:1603:A:H4'	1.97	0.46
3:B:1:U:H2'	3:B:2:G:C8	2.50	0.46
12:K:31:GLU:OE1	12:K:34:ARG:NH1	2.47	0.46
2:A:2647:U:H2'	2:A:2648:G:H8	1.80	0.46
11:J:14:ALA:HA	11:J:54:PRO:HA	1.96	0.46
11:J:55:ILE:HD12	11:J:74:PRO:HD3	1.96	0.46
2:A:151:C:H2'	2:A:152:A:H8	1.80	0.46
2:A:2798:U:H4'	2:A:2799:A:H5'	1.97	0.46
4:C:252:THR:HG23	4:C:253:LYS:HG3	1.97	0.46
15:N:61:GLY:HA3	15:N:106:ASP:O	2.15	0.46
23:V:74:ASN:HD21	23:V:99:ASN:HD21	1.63	0.46
2:A:833:A:H2'	2:A:834:G:C8	2.50	0.46
5:D:1:MET:HB3	5:D:205:PRO:HG2	1.98	0.46
11:J:11:LEU:HD22	11:J:24:VAL:HG23	1.98	0.46
24:W:2:PHE:HB2	24:W:61:LEU:HD22	1.97	0.46
34:h:461:LYS:HA	34:h:461:LYS:HD3	1.78	0.46
2:A:1029:A:N1	2:A:2465:C:O2'	2.46	0.46
3:B:48:U:H4'	17:P:100:HIS:HD2	1.79	0.46
18:Q:106:LYS:O	18:Q:109:ARG:NH2	2.49	0.46
26:Y:77:LYS:HA	26:Y:77:LYS:HD2	1.75	0.46
34:h:730:LEU:H	34:h:730:LEU:HD22	1.78	0.46
2:A:476:G:N1	2:A:479:A:OP2	2.48	0.46
2:A:1311:G:OP2	2:A:1311:G:N2	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:101:ASP:O	9:H:104:THR:OG1	2.34	0.46
16:O:79:LEU:HD23	16:O:83:LEU:HD12	1.97	0.46
25:X:25:ARG:HB3	25:X:29:GLU:HG2	1.97	0.46
2:A:526:A:O2'	2:A:2043:C:O2	2.30	0.46
4:C:155:ALA:HB2	4:C:162:VAL:HG23	1.97	0.46
34:h:178:THR:OG1	34:h:179:ASN:N	2.48	0.46
2:A:742:A:H2'	2:A:743:A:C8	2.51	0.46
2:A:1432:G:H2'	2:A:1433:A:C8	2.51	0.46
10:I:12:VAL:HG22	10:I:63:ALA:HB2	1.98	0.46
30:c:11:LEU:HD21	30:c:34:LEU:HD23	1.98	0.46
34:h:442:ILE:HG21	34:h:469:LEU:HD21	1.97	0.46
34:h:733:GLU:HG3	34:h:736:ARG:HD2	1.97	0.46
2:A:1429:G:H2'	2:A:1430:G:H8	1.81	0.46
11:J:12:GLN:HA	11:J:56:PRO:HA	1.99	0.46
2:A:2478:A:H5'	33:f:32:LYS:HD3	1.98	0.45
23:V:46:GLN:O	23:V:56:GLY:CA	2.64	0.45
34:h:688:ILE:HG21	34:h:736:ARG:HG2	1.98	0.45
2:A:355:U:H2'	2:A:356:G:C8	2.51	0.45
2:A:739:A:H1'	2:A:740:C:H5	1.81	0.45
2:A:1105:U:H2'	2:A:1106:G:C8	2.50	0.45
2:A:2127:G:H2'	2:A:2128:G:C8	2.51	0.45
9:H:9:VAL:HG23	9:H:12:LEU:HB2	1.99	0.45
3:B:8:C:O3'	17:P:25:ARG:NH1	2.45	0.45
2:A:2285:C:OP2	30:c:6:ARG:NE	2.50	0.45
2:A:2099:U:H3	2:A:2190:G:H1	1.64	0.45
2:A:2683:C:OP1	18:Q:51:ARG:NH2	2.42	0.45
5:D:132:ALA:HA	5:D:140:HIS:HD2	1.81	0.45
24:W:86:LEU:HD13	24:W:89:ILE:HD11	1.98	0.45
34:h:794:TYR:H	34:h:797:LYS:HE2	1.81	0.45
2:A:552:U:H2'	2:A:553:G:H8	1.81	0.45
2:A:1178:C:H2'	2:A:1179:G:H8	1.82	0.45
2:A:1181:U:H2'	2:A:1182:G:C8	2.52	0.45
24:W:38:LEU:HD21	24:W:65:VAL:HG11	1.98	0.45
30:c:17:THR:HG22	30:c:19:HIS:H	1.81	0.45
34:h:667:LEU:HD21	34:h:768:LEU:HD21	1.99	0.45
2:A:2039:U:H2'	2:A:2040:G:C8	2.51	0.45
2:A:2681:C:OP2	5:D:114:LYS:NZ	2.45	0.45
2:A:31:C:O2'	2:A:1238:G:OP1	2.34	0.45
31:d:12:ARG:HE	31:d:44:VAL:HG21	1.81	0.45
34:h:311:THR:HA	34:h:314:LEU:HD12	1.98	0.45
2:A:882:G:O6	2:A:894:U:O4	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1026:G:OP1	2:A:1134:A:O2'	2.32	0.45
6:E:83:VAL:HB	6:E:86:ALA:HB2	1.98	0.45
25:X:44:LYS:HB3	25:X:44:LYS:HE2	1.82	0.45
26:Y:56:MET:HE3	26:Y:56:MET:HB2	1.90	0.45
34:h:93:VAL:HG13	34:h:98:CYS:HB2	1.98	0.45
2:A:993:G:N3	20:S:91:GLN:NE2	2.63	0.45
2:A:1604:C:O2'	2:A:1610:A:N1	2.49	0.45
3:B:111:U:H2'	3:B:112:G:H8	1.82	0.45
13:L:70:ARG:HD3	13:L:76:VAL:HG22	1.98	0.45
15:N:33:LEU:HD13	15:N:117:PHE:HB3	1.97	0.45
15:N:62:LYS:O	15:N:105:MET:HA	2.17	0.45
18:Q:31:TRP:HB3	18:Q:38:LYS:HE2	1.99	0.45
27:Z:56:LEU:HA	27:Z:59:GLU:HG2	1.99	0.45
28:a:9:GLN:HB2	28:a:29:LEU:HD13	1.99	0.45
2:A:247:G:O6	32:e:12:LYS:NZ	2.40	0.44
2:A:296:U:H2'	2:A:297:G:C8	2.52	0.44
2:A:2100:G:O6	2:A:2189:U:O4	2.35	0.44
2:A:2135:A:N6	2:A:2156:G:O2'	2.50	0.44
11:J:113:LYS:O	11:J:117:MET:N	2.34	0.44
2:A:355:U:H2'	2:A:356:G:H8	1.82	0.44
2:A:414:C:H2'	2:A:415:A:C8	2.52	0.44
2:A:1385:A:O2'	2:A:1396:U:O2	2.33	0.44
2:A:1688:U:O2'	2:A:1700:A:N7	2.42	0.44
2:A:1980:G:O2'	2:A:1982:U:OP2	2.33	0.44
2:A:2898:U:H2'	2:A:2899:A:H8	1.82	0.44
4:C:212:ARG:HA	4:C:212:ARG:HD2	1.77	0.44
26:Y:12:PRO:HB3	26:Y:30:LEU:HD23	2.00	0.44
2:A:581:C:H2'	2:A:582:A:H8	1.82	0.44
2:A:1759:A:O2'	2:A:2714:G:O2'	2.35	0.44
2:A:1827:U:OP1	2:A:1971:U:O2'	2.34	0.44
2:A:2113:U:OP2	2:A:2115:G:N1	2.48	0.44
2:A:2861:U:H2'	2:A:2862:G:H8	1.83	0.44
3:B:60:C:H2'	3:B:61:G:H8	1.83	0.44
18:Q:14:LYS:NZ	18:Q:81:VAL:O	2.43	0.44
22:U:88:LYS:H	22:U:91:GLN:HE21	1.66	0.44
34:h:506:MET:HE3	34:h:574:ARG:HE	1.82	0.44
2:A:1590:A:H2'	2:A:1591:A:H8	1.81	0.44
23:V:13:VAL:HG21	23:V:39:ILE:HG21	1.99	0.44
34:h:515:LEU:HB3	34:h:548:VAL:HG11	2.00	0.44
30:c:30:LYS:HE2	30:c:30:LYS:HB2	1.88	0.44
29:b:28:LEU:HD23	29:b:28:LEU:HA	1.89	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:h:230:GLU:HB3	34:h:367:ASN:H	1.82	0.44
2:A:177:G:OP2	2:A:177:G:N2	2.47	0.44
2:A:483:A:H5''	23:V:47:LYS:HG2	1.98	0.44
2:A:832:U:H2'	2:A:833:A:H8	1.81	0.44
2:A:1068:G:O2'	2:A:1096:A:O2'	2.33	0.44
2:A:1275:A:N1	2:A:1295:C:O2'	2.48	0.44
2:A:2119:A:N7	2:A:2167:U:O2'	2.39	0.44
2:A:2347:C:O2'	30:c:21:TYR:OH	2.36	0.44
7:F:8:TYR:HB2	7:F:173:PHE:HZ	1.83	0.44
15:N:57:VAL:HG11	15:N:105:MET:HE1	1.99	0.44
18:Q:62:ARG:NH2	18:Q:71:GLU:OE1	2.51	0.44
2:A:84:A:N1	2:A:98:G:O2'	2.47	0.44
2:A:743:A:O2'	2:A:1659:G:OP1	2.31	0.44
2:A:1361:G:O2'	2:A:2215:C:O2'	2.34	0.44
7:F:68:THR:N	7:F:86:GLY:O	2.39	0.44
34:h:428:TYR:HB2	34:h:434:LYS:HB2	1.99	0.44
2:A:572:A:OP2	20:S:80:ARG:NH2	2.50	0.44
2:A:767:U:H2'	2:A:768:G:H8	1.82	0.44
2:A:793:A:OP2	2:A:2071:A:O2'	2.32	0.44
30:c:6:ARG:HG2	30:c:26:ASN:HB2	1.98	0.44
2:A:645:C:H2'	2:A:647:G:C8	2.53	0.43
2:A:1114:C:H2'	2:A:1115:G:C8	2.52	0.43
24:W:30:ILE:O	24:W:37:PRO:HA	2.18	0.43
34:h:771:LEU:O	34:h:775:TRP:HB3	2.18	0.43
2:A:2081:U:H2'	2:A:2082:A:H8	1.83	0.43
2:A:2333:A:H5'	2:A:2335:A:H1'	1.99	0.43
2:A:2627:G:O2'	2:A:2781:A:N1	2.41	0.43
10:I:52:MET:HE2	10:I:52:MET:HB2	1.87	0.43
11:J:58:VAL:HB	11:J:70:VAL:HB	2.00	0.43
15:N:20:LEU:HD13	24:W:81:PRO:HG2	2.00	0.43
2:A:5:A:H2'	2:A:6:A:C8	2.54	0.43
2:A:1316:U:H2'	2:A:1317:G:H8	1.83	0.43
2:A:2484:G:OP1	15:N:44:ARG:NH2	2.42	0.43
5:D:37:VAL:HG22	5:D:48:ILE:HG22	2.00	0.43
15:N:42:THR:HG22	15:N:93:VAL:HG12	1.99	0.43
22:U:3:ARG:HG2	22:U:5:GLU:HG2	2.00	0.43
34:h:60:LEU:HD11	34:h:118:LEU:HD22	2.01	0.43
2:A:2532:G:N2	2:A:2663:G:O2'	2.52	0.43
7:F:17:MET:HE3	7:F:17:MET:HB3	1.88	0.43
34:h:519:TRP:HA	34:h:522:GLU:HB2	1.99	0.43
2:A:721:A:H2'	2:A:722:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2140:G:H2'	2:A:2141:G:C8	2.53	0.43
2:A:2787:C:H1'	5:D:63:PRO:HG3	2.00	0.43
26:Y:18:ARG:HA	26:Y:18:ARG:HD2	1.80	0.43
2:A:1141:U:OP2	12:K:65:THR:OG1	2.35	0.43
2:A:1964:G:O2'	2:A:1967:C:OP2	2.27	0.43
3:B:90:C:H5''	15:N:18:ARG:HG2	1.99	0.43
20:S:78:ARG:HE	20:S:78:ARG:HB2	1.64	0.43
34:h:132:ASN:HD21	34:h:135:LEU:HG	1.83	0.43
2:A:1469:A:H2'	2:A:1470:A:H8	1.84	0.43
2:A:2316:G:H2'	2:A:2317:A:H8	1.83	0.43
34:h:37:LYS:HD2	34:h:37:LYS:HA	1.37	0.43
34:h:632:ARG:NH2	35:k:75:TRP:O	2.51	0.43
34:h:733:GLU:O	34:h:736:ARG:N	2.30	0.43
2:A:192:C:O2'	2:A:802:A:N3	2.49	0.43
2:A:302:C:H2'	2:A:303:G:H8	1.83	0.43
2:A:1168:G:H2'	2:A:1169:A:H8	1.84	0.43
2:A:1571:A:H2'	2:A:1572:A:C8	2.53	0.43
2:A:2898:U:H2'	2:A:2899:A:C8	2.54	0.43
14:M:64:PHE:HB3	32:e:25:LYS:HD2	2.00	0.43
28:a:23:THR:HG23	28:a:47:MET:HG2	2.01	0.43
30:c:33:LYS:HE2	30:c:33:LYS:HB2	1.88	0.43
2:A:143:C:H2'	2:A:144:A:C8	2.53	0.43
2:A:242:G:O2'	2:A:254:G:O6	2.35	0.43
2:A:832:U:H2'	2:A:833:A:C8	2.54	0.43
2:A:1592:C:H2'	2:A:1593:A:H8	1.83	0.43
2:A:2328:A:H2'	2:A:2329:U:C6	2.54	0.43
2:A:2467:C:OP1	33:f:8:LYS:NZ	2.41	0.43
2:A:2772:C:H5'	5:D:173:GLN:HE21	1.83	0.43
18:Q:30:VAL:HG13	18:Q:80:VAL:HG12	1.99	0.43
18:Q:100:LEU:HD11	18:Q:110:ILE:HD11	2.00	0.43
34:h:189:ASP:HB3	34:h:198:ARG:HD3	2.00	0.43
2:A:324:A:OP2	2:A:1205:A:N6	2.52	0.43
2:A:659:G:O2'	6:E:95:LYS:O	2.33	0.43
2:A:848:C:H2'	2:A:849:A:C8	2.54	0.43
2:A:1477:A:N6	2:A:1514:G:O2'	2.52	0.43
2:A:1645:G:H5''	2:A:1646:C:H5'	2.01	0.43
2:A:2117:A:H61	2:A:2171:A:H61	1.65	0.43
22:U:5:GLU:HA	22:U:8:LEU:HD12	2.01	0.43
34:h:155:GLY:O	34:h:175:THR:HA	2.19	0.43
34:h:211:VAL:HG22	34:h:391:THR:HB	2.00	0.43
2:A:1071:G:N2	2:A:1089:A:O2'	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1590:A:H2'	2:A:1591:A:C8	2.54	0.42
16:O:96:ARG:NH2	16:O:114:GLU:OE1	2.51	0.42
34:h:643:LYS:HD2	34:h:646:LEU:HD12	2.01	0.42
2:A:1056:G:H21	2:A:1103:A:H62	1.66	0.42
2:A:2656:U:O2	2:A:2665:A:N7	2.52	0.42
4:C:16:VAL:HG22	4:C:206:GLY:HA3	2.01	0.42
11:J:113:LYS:HG3	11:J:129:ILE:HD11	2.00	0.42
2:A:675:A:OP1	6:E:58:LYS:NZ	2.52	0.42
2:A:1734:G:H2'	2:A:1735:A:H8	1.85	0.42
2:A:2584:U:H3'	2:A:2585:U:H5''	1.99	0.42
10:I:111:ALA:HB3	10:I:118:ILE:HB	2.00	0.42
12:K:55:ILE:HA	12:K:123:LYS:O	2.20	0.42
18:Q:62:ARG:HB2	18:Q:71:GLU:HG2	2.01	0.42
21:T:29:VAL:HB	21:T:55:ILE:HD11	2.01	0.42
34:h:730:LEU:HD23	34:h:731:HIS:H	1.83	0.42
2:A:296:U:H2'	2:A:297:G:H8	1.83	0.42
2:A:596:U:H2'	2:A:597:G:H8	1.85	0.42
2:A:861:A:N3	3:B:79:G:O2'	2.53	0.42
2:A:1244:A:O2'	6:E:29:HIS:NE2	2.42	0.42
2:A:1715:G:O2'	2:A:1743:G:O6	2.27	0.42
4:C:24:LEU:HD23	4:C:83:TYR:HB2	2.02	0.42
14:M:57:LEU:HD22	32:e:54:ASP:HB3	2.00	0.42
15:N:74:THR:HA	15:N:88:ASN:O	2.19	0.42
25:X:65:GLY:HA3	25:X:83:GLU:O	2.19	0.42
30:c:11:LEU:HA	30:c:50:LYS:O	2.19	0.42
34:h:287:VAL:HG12	34:h:293:ASP:HB2	2.01	0.42
2:A:1592:C:H2'	2:A:1593:A:C8	2.55	0.42
2:A:2718:G:O2'	2:A:2847:U:OP1	2.37	0.42
4:C:21:ASN:HB3	4:C:24:LEU:HD13	2.01	0.42
7:F:14:LYS:HB3	7:F:14:LYS:HE2	1.77	0.42
22:U:51:PHE:HB3	35:k:63:LEU:HD22	2.00	0.42
33:f:15:LYS:HB3	33:f:15:LYS:HE2	1.82	0.42
35:k:72:ALA:HA	35:k:75:TRP:HB3	2.00	0.42
2:A:1000:A:OP2	2:A:1154:G:N1	2.39	0.42
2:A:2591:C:H2'	2:A:2592:G:H8	1.85	0.42
2:A:59:U:O2'	2:A:74:A:OP2	2.30	0.42
2:A:372:G:O2'	2:A:400:G:O6	2.30	0.42
2:A:880:G:H2'	2:A:881:G:H8	1.84	0.42
2:A:2070:A:H2'	2:A:2071:A:C8	2.54	0.42
2:A:2229:U:H2'	2:A:2230:G:C8	2.54	0.42
15:N:26:VAL:HG13	15:N:104:GLU:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:57:VAL:HG12	15:N:112:LEU:HG	2.02	0.42
24:W:73:LYS:HE2	24:W:73:LYS:HB3	1.76	0.42
34:h:130:THR:OG1	34:h:132:ASN:O	2.38	0.42
2:A:219:A:N3	2:A:234:U:O2'	2.44	0.42
2:A:968:C:H2'	2:A:969:G:H8	1.84	0.42
2:A:1096:A:H61	11:J:30:GLN:HE22	1.68	0.42
2:A:1153:C:H5'	19:R:76:TYR:HE2	1.85	0.42
2:A:1435:G:H2'	2:A:1436:G:C8	2.55	0.42
2:A:1563:U:H2'	2:A:1564:C:C6	2.55	0.42
5:D:56:LYS:HB2	5:D:59:ARG:HB2	2.02	0.42
9:H:68:ARG:HH21	9:H:110:VAL:HG12	1.84	0.42
10:I:54:VAL:HG22	10:I:81:LEU:HD13	2.00	0.42
34:h:328:VAL:HG11	34:h:363:VAL:HG22	2.01	0.42
2:A:2199:A:N6	2:A:2224:G:O2'	2.52	0.42
4:C:23:GLU:HG3	4:C:81:LEU:HD12	2.02	0.42
9:H:41:LYS:HE3	9:H:41:LYS:HB2	1.86	0.42
25:X:50:ASN:HB2	25:X:82:ILE:HB	2.01	0.42
27:Z:34:SER:HA	34:h:1:MET:HE2	2.00	0.42
2:A:160:A:N3	2:A:2208:C:O2'	2.45	0.42
2:A:376:G:H2'	2:A:377:G:H8	1.85	0.42
2:A:1045:C:OP1	2:A:1046:A:O2'	2.32	0.42
2:A:1045:C:OP1	10:I:8:LYS:NZ	2.53	0.42
2:A:1710:G:H2'	2:A:1711:A:C8	2.55	0.42
6:E:178:VAL:HG23	14:M:3:LEU:HD21	2.01	0.42
30:c:23:THR:OG1	30:c:24:THR:N	2.53	0.42
34:h:479:LEU:HD22	34:h:487:GLU:HG2	2.02	0.42
34:h:643:LYS:HD2	34:h:643:LYS:HA	1.77	0.42
34:h:791:LEU:HD21	34:h:792:ARG:HH11	1.84	0.42
2:A:581:C:H2'	2:A:582:A:C8	2.55	0.41
2:A:665:U:H2'	2:A:666:A:H8	1.85	0.41
2:A:1227:G:OP2	19:R:16:LYS:NZ	2.52	0.41
2:A:2086:U:H2'	2:A:2087:G:C8	2.55	0.41
2:A:2241:A:H2'	2:A:2242:G:C8	2.55	0.41
3:B:93:C:H2'	3:B:94:A:H8	1.85	0.41
7:F:36:LEU:HD22	7:F:154:ILE:HG12	2.02	0.41
21:T:23:LEU:O	21:T:27:LYS:NZ	2.44	0.41
34:h:3:ILE:HD12	35:k:72:ALA:HB3	2.02	0.41
2:A:5:A:H2'	2:A:6:A:H8	1.84	0.41
2:A:997:G:OP2	19:R:58:ARG:NH1	2.53	0.41
2:A:2031:A:N3	2:A:2455:G:O2'	2.47	0.41
2:A:2591:C:H2'	2:A:2592:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:h:714:PHE:HE1	34:h:823:ILE:HG22	1.85	0.41
11:J:36:MET:HE3	11:J:36:MET:HB3	1.91	0.41
2:A:1447:C:H2'	2:A:1448:G:H8	1.84	0.41
13:L:13:ASN:OD1	13:L:97:THR:N	2.54	0.41
22:U:24:MET:HE1	22:U:30:ILE:HG22	2.02	0.41
23:V:46:GLN:O	23:V:56:GLY:HA2	2.20	0.41
30:c:13:SER:HB3	30:c:49:TYR:CZ	2.56	0.41
2:A:347:A:H2'	2:A:348:A:C8	2.56	0.41
2:A:1447:C:H2'	2:A:1448:G:C8	2.56	0.41
8:G:86:LYS:HG2	8:G:132:VAL:HG22	2.01	0.41
9:H:26:ALA:HA	9:H:30:LEU:HB2	2.01	0.41
19:R:80:ILE:HD13	19:R:80:ILE:HA	1.93	0.41
34:h:1:MET:HE3	34:h:2:LEU:H	1.85	0.41
34:h:443:LYS:HD2	34:h:443:LYS:HA	1.83	0.41
2:A:1077:A:O2'	11:J:94:ASN:OD1	2.37	0.41
2:A:2339:C:H2'	2:A:2340:A:C8	2.56	0.41
2:A:2419:U:H4'	30:c:22:THR:HG21	2.02	0.41
2:A:2757:A:N1	8:G:67:THR:OG1	2.47	0.41
3:B:54:G:H21	7:F:26:MET:HE3	1.84	0.41
4:C:154:LEU:HD13	4:C:176:LEU:HD21	2.02	0.41
7:F:14:LYS:HA	7:F:17:MET:HB2	2.01	0.41
2:A:782:A:N7	4:C:220:VAL:HG21	2.36	0.41
2:A:1363:C:O2'	2:A:1809:A:N3	2.45	0.41
2:A:2279:G:N7	25:X:14:ARG:NH2	2.54	0.41
10:I:92:ALA:HA	10:I:95:LEU:HB3	2.02	0.41
2:A:358:U:H2'	2:A:359:G:C8	2.55	0.41
2:A:926:G:H2'	2:A:927:A:C8	2.55	0.41
10:I:28:ALA:HB3	10:I:81:LEU:HB3	2.02	0.41
34:h:71:VAL:O	34:h:74:ALA:HB3	2.20	0.41
34:h:305:MET:HE3	34:h:781:ALA:HB2	2.03	0.41
34:h:400:GLU:O	34:h:404:ILE:HG13	2.21	0.41
2:A:4:U:H2'	2:A:5:A:C8	2.56	0.41
2:A:438:G:H2'	2:A:439:A:C8	2.56	0.41
2:A:631:A:N3	2:A:2415:G:O2'	2.48	0.41
2:A:903:C:H2'	2:A:904:G:H8	1.86	0.41
2:A:927:A:H2'	2:A:928:A:C8	2.55	0.41
2:A:1123:C:H2'	2:A:1124:G:H8	1.85	0.41
2:A:1681:G:O2'	2:A:1762:A:N3	2.48	0.41
2:A:2857:G:N2	2:A:2860:A:OP2	2.44	0.41
8:G:2:SER:OG	8:G:3:ARG:N	2.52	0.41
9:H:90:LEU:HD12	9:H:90:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:4:LYS:HE2	17:P:8:ILE:HD11	2.03	0.41
29:b:29:SER:OG	29:b:40:ARG:NH1	2.49	0.41
34:h:593:ALA:O	34:h:596:ARG:HB2	2.21	0.41
34:h:630:ALA:HA	34:h:633:LYS:HE3	2.01	0.41
2:A:69:C:O2	2:A:73:A:O2'	2.38	0.41
2:A:133:U:H2'	2:A:134:G:C8	2.56	0.41
2:A:1028:A:N3	2:A:2486:C:O2'	2.39	0.41
2:A:1452:G:H22	2:A:1457:U:H2'	1.86	0.41
2:A:1636:U:H2'	2:A:1637:A:C8	2.56	0.41
2:A:1667:G:O2'	2:A:1991:U:O4	2.33	0.41
2:A:2076:U:OP2	2:A:2238:G:N2	2.40	0.41
3:B:28:C:H2'	3:B:29:A:C8	2.56	0.41
4:C:232:HIS:HA	4:C:242:LYS:HD2	2.03	0.41
14:M:9:ALA:HB3	14:M:12:SER:HB3	2.02	0.41
34:h:22:ARG:HA	34:h:22:ARG:HD3	1.83	0.41
2:A:288:U:H2'	2:A:289:G:H8	1.86	0.40
2:A:589:U:H2'	2:A:590:A:C8	2.56	0.40
2:A:598:U:H2'	2:A:599:A:H8	1.85	0.40
2:A:796:C:H2'	2:A:797:G:C8	2.57	0.40
6:E:97:ASN:ND2	6:E:100:MET:SD	2.94	0.40
9:H:72:ILE:HG13	9:H:108:VAL:HG11	2.03	0.40
10:I:97:LYS:HD2	10:I:123:ILE:HB	2.01	0.40
13:L:94:PRO:HD2	13:L:114:LYS:HD2	2.02	0.40
34:h:733:GLU:O	34:h:735:LEU:N	2.54	0.40
2:A:837:C:N3	2:A:941:A:N6	2.69	0.40
2:A:1076:C:H2'	2:A:1077:A:C8	2.56	0.40
2:A:1263:U:OP1	29:b:13:ARG:NH1	2.43	0.40
2:A:1510:G:H2'	2:A:1511:G:H8	1.87	0.40
2:A:2627:G:N2	2:A:2777:G:OP2	2.54	0.40
5:D:25:THR:OG1	5:D:191:GLY:O	2.34	0.40
9:H:58:LEU:HA	9:H:58:LEU:HD23	1.85	0.40
9:H:78:VAL:O	9:H:144:VAL:HA	2.21	0.40
12:K:32:LEU:HD22	12:K:54:ILE:HG21	2.02	0.40
34:h:304:ILE:HG12	34:h:785:LEU:HD13	2.04	0.40
34:h:695:GLN:OE1	34:h:732:GLU:OE2	2.40	0.40
2:A:287:G:H2'	2:A:288:U:C6	2.55	0.40
2:A:550:C:H2'	2:A:551:G:H8	1.86	0.40
2:A:1278:C:H2'	2:A:1279:G:C8	2.55	0.40
2:A:1435:G:H2'	2:A:1436:G:H8	1.86	0.40
2:A:1730:C:O2	2:A:1731:G:N1	2.54	0.40
2:A:2087:G:H2'	2:A:2088:A:C8	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2427:C:H5'	2:A:2429:G:H5'	2.03	0.40
4:C:37:ASN:HB2	4:C:62:TYR:HB2	2.03	0.40
4:C:153:GLN:HA	4:C:156:ARG:HH21	1.86	0.40
11:J:47:ASP:OD1	11:J:47:ASP:N	2.54	0.40
13:L:12:ASP:OD1	13:L:14:SER:OG	2.35	0.40
22:U:54:GLU:N	22:U:91:GLN:OE1	2.50	0.40
34:h:25:VAL:O	34:h:29:ASN:ND2	2.55	0.40
34:h:38:LEU:HD22	34:h:77:ARG:HB3	2.04	0.40
34:h:376:THR:OG1	34:h:378:GLN:OE1	2.29	0.40
2:A:1:G:H2'	2:A:2:G:H8	1.86	0.40
2:A:671:C:H2'	2:A:672:C:H6	1.86	0.40
2:A:910:A:H2'	2:A:911:A:C8	2.56	0.40
2:A:1288:G:OP2	2:A:1288:G:N2	2.40	0.40
2:A:1380:G:O2'	2:A:1569:A:N6	2.54	0.40
2:A:2099:U:O2	2:A:2190:G:N2	2.41	0.40
2:A:2514:U:H2'	2:A:2515:C:C6	2.56	0.40
2:A:2698:U:H2'	2:A:2699:C:C6	2.57	0.40
12:K:7:LYS:HA	12:K:8:PRO:HD3	1.93	0.40
18:Q:75:GLN:HB2	18:Q:78:SER:HB2	2.03	0.40
34:h:692:ILE:HG23	34:h:701:TRP:CD1	2.56	0.40
2:A:414:C:H2'	2:A:415:A:H8	1.86	0.40
2:A:675:A:N3	2:A:2443:C:O2'	2.53	0.40
2:A:1571:A:H2'	2:A:1572:A:H8	1.87	0.40
2:A:2087:G:H2'	2:A:2088:A:H8	1.87	0.40
2:A:2189:U:H2'	2:A:2190:G:H8	1.87	0.40
3:B:49:C:H2'	3:B:50:A:H8	1.87	0.40
4:C:107:PRO:HD2	4:C:110:LEU:HD22	2.04	0.40
8:G:17:VAL:HG11	8:G:50:LEU:HD11	2.04	0.40
9:H:57:LYS:HE2	9:H:57:LYS:HB3	1.85	0.40
15:N:105:MET:HE2	15:N:108:VAL:HG21	2.04	0.40
16:O:65:LEU:HD12	16:O:65:LEU:HA	1.97	0.40
23:V:13:VAL:HG22	23:V:70:VAL:HG12	2.03	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	
4	C	270/273 (99%)	262 (97%)	8 (3%)	0	100	100
5	D	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
6	E	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
7	F	176/179 (98%)	169 (96%)	7 (4%)	0	100	100
8	G	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
9	H	147/149 (99%)	141 (96%)	6 (4%)	0	100	100
10	I	123/165 (74%)	114 (93%)	7 (6%)	2 (2%)	7	30
11	J	132/142 (93%)	122 (92%)	10 (8%)	0	100	100
12	K	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
13	L	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
14	M	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
15	N	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
16	O	123/127 (97%)	119 (97%)	4 (3%)	0	100	100
17	P	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
18	Q	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
19	R	115/118 (98%)	115 (100%)	0	0	100	100
20	S	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
21	T	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
22	U	90/100 (90%)	86 (96%)	4 (4%)	0	100	100
23	V	101/104 (97%)	94 (93%)	7 (7%)	0	100	100
24	W	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
25	X	74/85 (87%)	70 (95%)	4 (5%)	0	100	100
26	Y	75/78 (96%)	75 (100%)	0	0	100	100
27	Z	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
28	a	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
29	b	54/57 (95%)	54 (100%)	0	0	100	100
30	c	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
31	d	44/46 (96%)	44 (100%)	0	0	100	100
32	e	62/65 (95%)	55 (89%)	5 (8%)	2 (3%)	3	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	f	36/38 (95%)	36 (100%)	0	0	100	100
34	h	836/838 (100%)	753 (90%)	75 (9%)	8 (1%)	12	41
35	k	53/57 (93%)	46 (87%)	7 (13%)	0	100	100
All	All	4321/4469 (97%)	4123 (95%)	186 (4%)	12 (0%)	37	67

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	e	32	ILE
34	h	734	THR
32	e	33	LEU
34	h	38	LEU
34	h	258	GLN
34	h	231	ASP
34	h	257	PHE
34	h	801	GLN
34	h	404	ILE
34	h	287	VAL
10	I	108	VAL
10	I	67	THR

5.3.2 Protein sidechains [i](#)

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	C	216/218 (99%)	214 (99%)	2 (1%)	70	80
5	D	164/164 (100%)	164 (100%)	0	100	100
6	E	165/165 (100%)	165 (100%)	0	100	100
7	F	148/150 (99%)	146 (99%)	2 (1%)	59	76
8	G	137/138 (99%)	136 (99%)	1 (1%)	76	82
9	H	114/114 (100%)	113 (99%)	1 (1%)	70	80
10	I	95/123 (77%)	92 (97%)	3 (3%)	34	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	J	104/110 (94%)	102 (98%)	2 (2%)	50	73
12	K	116/116 (100%)	116 (100%)	0	100	100
13	L	104/104 (100%)	104 (100%)	0	100	100
14	M	103/103 (100%)	103 (100%)	0	100	100
15	N	109/109 (100%)	109 (100%)	0	100	100
16	O	102/103 (99%)	101 (99%)	1 (1%)	68	79
17	P	87/87 (100%)	87 (100%)	0	100	100
18	Q	99/100 (99%)	99 (100%)	0	100	100
19	R	89/90 (99%)	89 (100%)	0	100	100
20	S	84/84 (100%)	83 (99%)	1 (1%)	63	78
21	T	93/93 (100%)	93 (100%)	0	100	100
22	U	79/84 (94%)	79 (100%)	0	100	100
23	V	83/85 (98%)	83 (100%)	0	100	100
24	W	78/78 (100%)	78 (100%)	0	100	100
25	X	57/63 (90%)	57 (100%)	0	100	100
26	Y	67/68 (98%)	67 (100%)	0	100	100
27	Z	54/55 (98%)	54 (100%)	0	100	100
28	a	48/49 (98%)	47 (98%)	1 (2%)	47	71
29	b	47/48 (98%)	47 (100%)	0	100	100
30	c	45/49 (92%)	44 (98%)	1 (2%)	45	71
31	d	38/38 (100%)	38 (100%)	0	100	100
32	e	51/52 (98%)	51 (100%)	0	100	100
33	f	34/34 (100%)	34 (100%)	0	100	100
34	h	714/714 (100%)	703 (98%)	11 (2%)	57	75
35	k	21/30 (70%)	21 (100%)	0	100	100
All	All	3545/3618 (98%)	3519 (99%)	26 (1%)	73	82

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	C	3	VAL
4	C	174	LEU
7	F	74	VAL

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Mol	Chain	Res	Type
7	F	149	VAL
8	G	49	THR
9	H	124	THR
10	I	64	VAL
10	I	72	LEU
10	I	108	VAL
11	J	46	THR
11	J	80	LEU
16	O	57	THR
20	S	63	VAL
28	a	4	THR
30	c	47	VAL
34	h	35	MET
34	h	36	GLU
34	h	37	LYS
34	h	129	VAL
34	h	148	GLU
34	h	272	VAL
34	h	396	THR
34	h	477	ASN
34	h	730	LEU
34	h	789	ILE
34	h	818	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
4	C	115	GLN
4	C	243	HIS
4	C	260	ASN
5	D	42	ASN
5	D	173	GLN
6	E	9	GLN
6	E	136	GLN
7	F	23	ASN
7	F	63	GLN
8	G	38	ASN
8	G	73	ASN
8	G	101	ASN
8	G	116	GLN
9	H	33	GLN
9	H	66	ASN

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Mol	Chain	Res	Type
9	H	128	HIS
9	H	135	HIS
9	H	145	ASN
10	I	103	ASN
11	J	12	GLN
11	J	19	ASN
11	J	30	GLN
13	L	3	GLN
14	M	54	GLN
15	N	3	GLN
15	N	22	GLN
16	O	18	GLN
16	O	62	ASN
18	Q	41	GLN
18	Q	75	GLN
19	R	44	GLN
19	R	81	ASN
20	S	82	HIS
20	S	89	HIS
20	S	91	GLN
22	U	48	GLN
22	U	70	HIS
22	U	92	ASN
23	V	74	ASN
24	W	49	ASN
26	Y	6	GLN
26	Y	34	HIS
27	Z	27	ASN
27	Z	39	GLN
30	c	26	ASN
33	f	13	ASN
34	h	29	ASN
34	h	87	GLN
34	h	258	GLN
34	h	415	ASN
34	h	476	HIS
34	h	520	GLN
34	h	533	GLN
34	h	569	ASN
34	h	629	ASN
34	h	638	ASN
34	h	731	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	2/3 (66%)	1 (50%)	0
2	A	2878/2883 (99%)	446 (15%)	8 (0%)
3	B	119/120 (99%)	14 (11%)	0
All	All	2999/3006 (99%)	461 (15%)	8 (0%)

All (461) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	76	A
2	A	10	A
2	A	12	U
2	A	15	G
2	A	34	U
2	A	35	G
2	A	46	G
2	A	58	G
2	A	63	A
2	A	71	A
2	A	74	A
2	A	75	G
2	A	84	A
2	A	91	A
2	A	101	A
2	A	102	U
2	A	118	A
2	A	119	A
2	A	120	U
2	A	125	A
2	A	136	G
2	A	137	U
2	A	138	U
2	A	139	U
2	A	141	G
2	A	163	C
2	A	165	A
2	A	181	A
2	A	196	A
2	A	199	A
2	A	215	G
2	A	216	A
2	A	221	A

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Mol	Chain	Res	Type
2	A	222	A
2	A	226	A
2	A	248	G
2	A	266	G
2	A	272	A
2	A	276	U
2	A	277	G
2	A	279	A
2	A	302	C
2	A	311	A
2	A	329	G
2	A	330	A
2	A	353	C
2	A	354	A
2	A	361	G
2	A	362	A
2	A	372	G
2	A	386	G
2	A	396	G
2	A	399	U
2	A	404	A
2	A	405	U
2	A	406	G
2	A	411	G
2	A	412	A
2	A	420	C
2	A	424	G
2	A	435	C
2	A	455	C
2	A	467	G
2	A	477	A
2	A	479	A
2	A	481	G
2	A	491	G
2	A	505	A
2	A	509	C
2	A	529	A
2	A	530	G
2	A	531	C
2	A	532	A
2	A	543	G
2	A	549	G

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Mol	Chain	Res	Type
2	A	551	G
2	A	563	A
2	A	573	U
2	A	575	A
2	A	592	A
2	A	603	A
2	A	613	A
2	A	614	A
2	A	615	U
2	A	621	A
2	A	627	A
2	A	637	A
2	A	645	C
2	A	646	U
2	A	647	G
2	A	651	G
2	A	653	U
2	A	654	A
2	A	655	A
2	A	686	U
2	A	714	U
2	A	717	C
2	A	726	G
2	A	730	A
2	A	747	U
2	A	762	U
2	A	764	A
2	A	765	C
2	A	775	G
2	A	776	G
2	A	777	G
2	A	782	A
2	A	784	G
2	A	785	G
2	A	790	U
2	A	791	C
2	A	792	A
2	A	800	A
2	A	801	G
2	A	805	G
2	A	811	U
2	A	812	C

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Mol	Chain	Res	Type
2	A	827	U
2	A	828	U
2	A	831	G
2	A	845	A
2	A	846	U
2	A	847	U
2	A	859	G
2	A	869	G
2	A	878	A
2	A	896	A
2	A	897	C
2	A	907	G
2	A	910	A
2	A	934	U
2	A	946	C
2	A	953	G
2	A	961	C
2	A	973	A
2	A	974	G
2	A	983	A
2	A	989	G
2	A	996	A
2	A	1005	C
2	A	1009	A
2	A	1012	U
2	A	1013	C
2	A	1023	U
2	A	1025	G
2	A	1026	G
2	A	1033	U
2	A	1040	A
2	A	1046	A
2	A	1060	U
2	A	1069	A
2	A	1070	A
2	A	1071	G
2	A	1073	A
2	A	1074	G
2	A	1083	U
2	A	1084	A
2	A	1087	G
2	A	1088	A

Continued on next page...

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Mol	Chain	Res	Type
2	A	1097	U
2	A	1101	U
2	A	1112	G
2	A	1122	G
2	A	1128	G
2	A	1132	U
2	A	1133	A
2	A	1135	C
2	A	1142	A
2	A	1155	A
2	A	1173	U
2	A	1178	C
2	A	1212	G
2	A	1218	G
2	A	1227	G
2	A	1236	G
2	A	1238	G
2	A	1247	A
2	A	1250	G
2	A	1253	A
2	A	1256	G
2	A	1271	G
2	A	1272	A
2	A	1275	A
2	A	1300	G
2	A	1301	A
2	A	1321	A
2	A	1329	U
2	A	1345	C
2	A	1352	U
2	A	1360	G
2	A	1365	A
2	A	1378	A
2	A	1379	U
2	A	1383	A
2	A	1416	G
2	A	1417	C
2	A	1421	G
2	A	1427	A
2	A	1428	C
2	A	1434	A
2	A	1435	G

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Mol	Chain	Res	Type
2	A	1437	C
2	A	1451	C
2	A	1453	A
2	A	1460	U
2	A	1482	G
2	A	1491	G
2	A	1493	C
2	A	1494	A
2	A	1495	A
2	A	1497	U
2	A	1508	A
2	A	1510	G
2	A	1515	A
2	A	1524	G
2	A	1533	C
2	A	1534	U
2	A	1536	C
2	A	1537	G
2	A	1557	C
2	A	1558	C
2	A	1566	A
2	A	1569	A
2	A	1578	U
2	A	1583	A
2	A	1584	U
2	A	1585	C
2	A	1607	C
2	A	1608	A
2	A	1610	A
2	A	1634	A
2	A	1647	U
2	A	1648	U
2	A	1649	G
2	A	1669	A
2	A	1674	G
2	A	1698	A
2	A	1715	G
2	A	1729	U
2	A	1730	C
2	A	1732	C
2	A	1738	G
2	A	1756	G

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Mol	Chain	Res	Type
2	A	1757	A
2	A	1758	U
2	A	1764	C
2	A	1773	A
2	A	1781	U
2	A	1782	U
2	A	1784	A
2	A	1800	C
2	A	1801	A
2	A	1802	A
2	A	1808	A
2	A	1811	G
2	A	1816	C
2	A	1829	A
2	A	1870	C
2	A	1871	A
2	A	1872	A
2	A	1873	G
2	A	1906	G
2	A	1929	G
2	A	1936	A
2	A	1938	A
2	A	1939	U
2	A	1955	U
2	A	1967	C
2	A	1970	A
2	A	1971	U
2	A	1972	G
2	A	1982	U
2	A	1991	U
2	A	1992	G
2	A	1993	U
2	A	1997	C
2	A	2020	A
2	A	2023	C
2	A	2030	A
2	A	2031	A
2	A	2033	A
2	A	2043	C
2	A	2055	C
2	A	2056	G
2	A	2060	A

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Mol	Chain	Res	Type
2	A	2061	G
2	A	2062	A
2	A	2069	G
2	A	2093	G
2	A	2097	A
2	A	2104	C
2	A	2106	U
2	A	2108	A
2	A	2111	U
2	A	2112	G
2	A	2113	U
2	A	2114	A
2	A	2115	G
2	A	2117	A
2	A	2118	U
2	A	2119	A
2	A	2120	G
2	A	2123	G
2	A	2125	G
2	A	2126	A
2	A	2128	G
2	A	2130	U
2	A	2131	U
2	A	2132	U
2	A	2133	G
2	A	2134	A
2	A	2137	U
2	A	2145	C
2	A	2146	C
2	A	2148	G
2	A	2158	A
2	A	2159	G
2	A	2161	C
2	A	2162	G
2	A	2163	A
2	A	2164	C
2	A	2165	C
2	A	2167	U
2	A	2168	G
2	A	2169	A
2	A	2170	A
2	A	2171	A

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Mol	Chain	Res	Type
2	A	2172	U
2	A	2173	A
2	A	2177	C
2	A	2179	C
2	A	2184	A
2	A	2186	G
2	A	2187	U
2	A	2188	U
2	A	2191	A
2	A	2192	U
2	A	2198	A
2	A	2199	A
2	A	2203	U
2	A	2204	G
2	A	2210	U
2	A	2211	A
2	A	2223	G
2	A	2225	A
2	A	2238	G
2	A	2239	G
2	A	2266	A
2	A	2278	A
2	A	2279	G
2	A	2283	C
2	A	2287	A
2	A	2288	A
2	A	2305	U
2	A	2308	G
2	A	2309	A
2	A	2310	C
2	A	2322	A
2	A	2325	G
2	A	2333	A
2	A	2334	U
2	A	2347	C
2	A	2350	C
2	A	2361	G
2	A	2383	G
2	A	2385	C
2	A	2391	G
2	A	2402	U
2	A	2406	A

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Mol	Chain	Res	Type
2	A	2422	C
2	A	2424	C
2	A	2425	A
2	A	2428	G
2	A	2429	G
2	A	2430	A
2	A	2431	U
2	A	2432	A
2	A	2434	A
2	A	2435	A
2	A	2441	U
2	A	2447	G
2	A	2448	A
2	A	2470	G
2	A	2476	A
2	A	2478	A
2	A	2491	U
2	A	2494	G
2	A	2498	C
2	A	2502	G
2	A	2505	G
2	A	2518	A
2	A	2520	C
2	A	2529	G
2	A	2547	A
2	A	2562	U
2	A	2566	A
2	A	2567	G
2	A	2572	A
2	A	2585	U
2	A	2586	U
2	A	2602	A
2	A	2603	G
2	A	2609	U
2	A	2613	U
2	A	2615	U
2	A	2621	G
2	A	2629	U
2	A	2646	C
2	A	2654	A
2	A	2663	G
2	A	2682	A

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Mol	Chain	Res	Type
2	A	2684	U
2	A	2689	U
2	A	2690	U
2	A	2714	G
2	A	2716	C
2	A	2726	A
2	A	2733	A
2	A	2739	U
2	A	2744	G
2	A	2748	A
2	A	2757	A
2	A	2765	A
2	A	2778	A
2	A	2779	U
2	A	2791	G
2	A	2792	A
2	A	2798	U
2	A	2799	A
2	A	2800	A
2	A	2818	U
2	A	2820	A
2	A	2825	G
2	A	2833	U
2	A	2835	A
2	A	2836	U
2	A	2849	U
2	A	2861	U
2	A	2867	G
2	A	2872	A
2	A	2873	A
2	A	2879	A
2	A	2880	C
2	A	2883	A
2	A	2884	U
2	A	2886	A
2	A	2891	U
3	B	9	G
3	B	13	G
3	B	24	G
3	B	35	C
3	B	41	G
3	B	56	G

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Mol	Chain	Res	Type
3	B	66	A
3	B	67	G
3	B	88	C
3	B	89	U
3	B	90	C
3	B	105	G
3	B	109	A
3	B	120	U

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	613	A
2	A	784	G
2	A	1494	A
2	A	2112	G
2	A	2127	G
2	A	2158	A
2	A	2602	A
2	A	2756	U

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 69 ligands modelled in this entry, 69 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	A	4
35	k	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	k	76:GLN	C	109:ALA	N	27.78
1	A	882:G	O3'	894:U	P	15.86
1	A	1912:A	O3'	1917:U	P	14.04
1	A	545:U	O3'	548:G	P	13.58
1	A	1173:U	O3'	1177:G	P	13.39

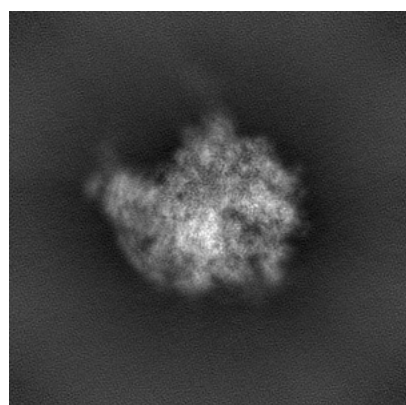
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10073. These allow visual inspection of the internal detail of the map and identification of artifacts.

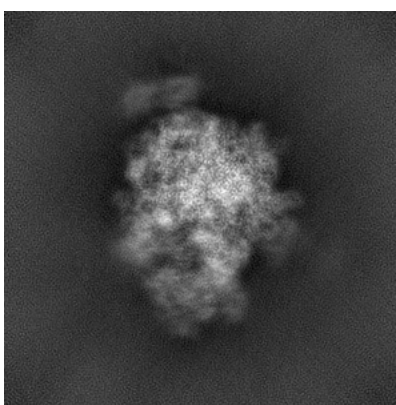
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

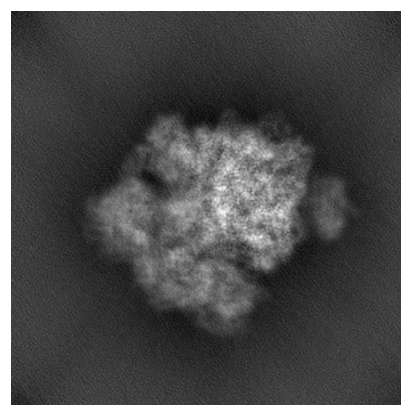
6.1.1 Primary map



X



Y

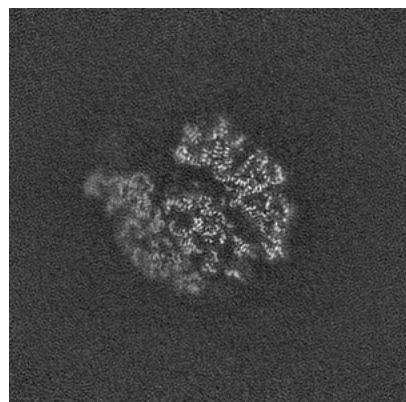


Z

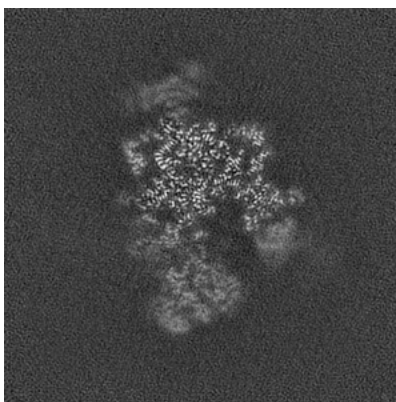
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

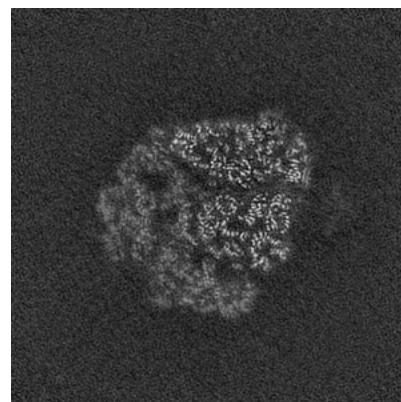
6.2.1 Primary map



X Index: 160



Y Index: 160

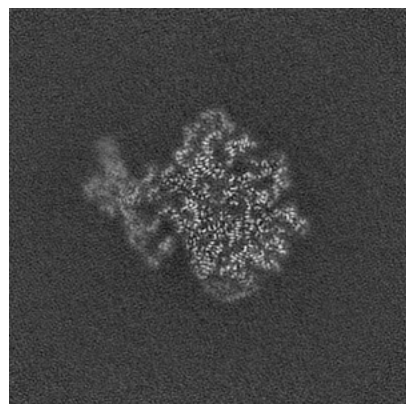


Z Index: 160

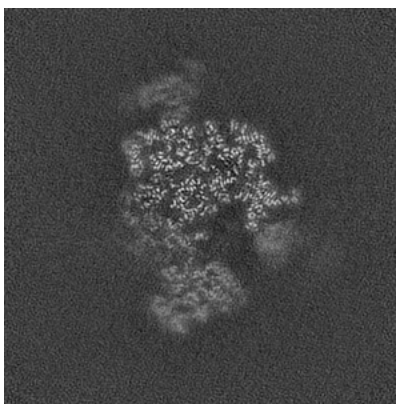
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

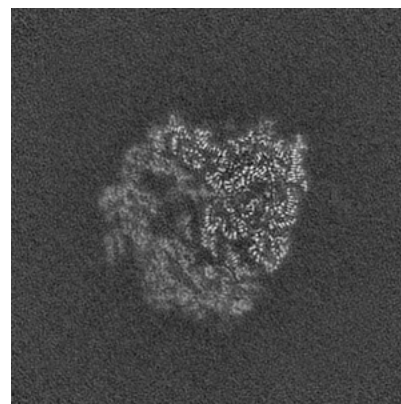
6.3.1 Primary map



X Index: 170



Y Index: 157

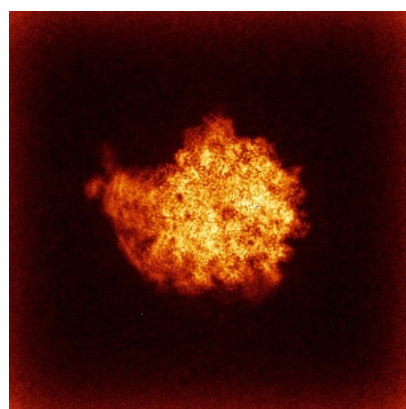


Z Index: 165

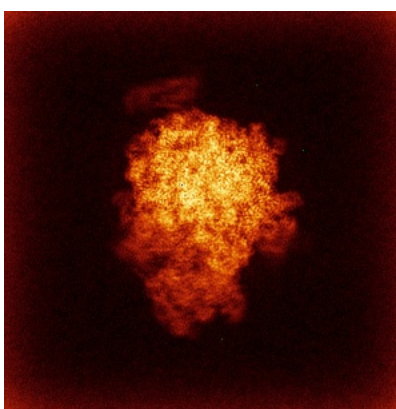
The images above show the largest variance slices of the map in three orthogonal directions.

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

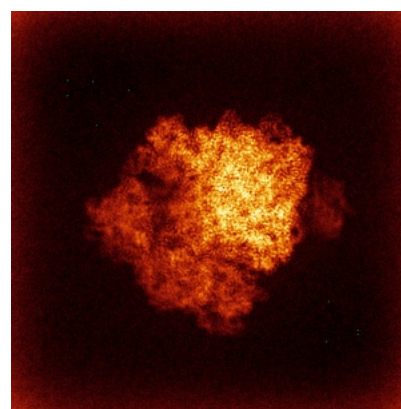
6.4.1 Primary map



X



Y

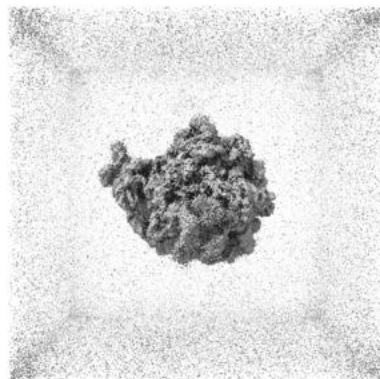


Z

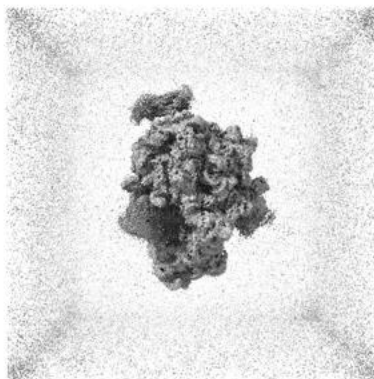
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

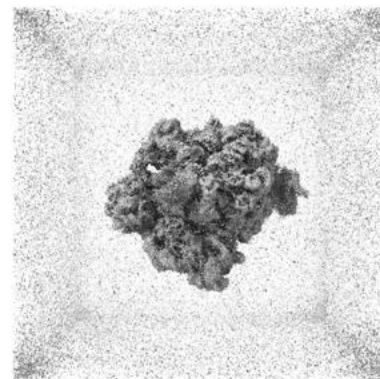
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.82. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

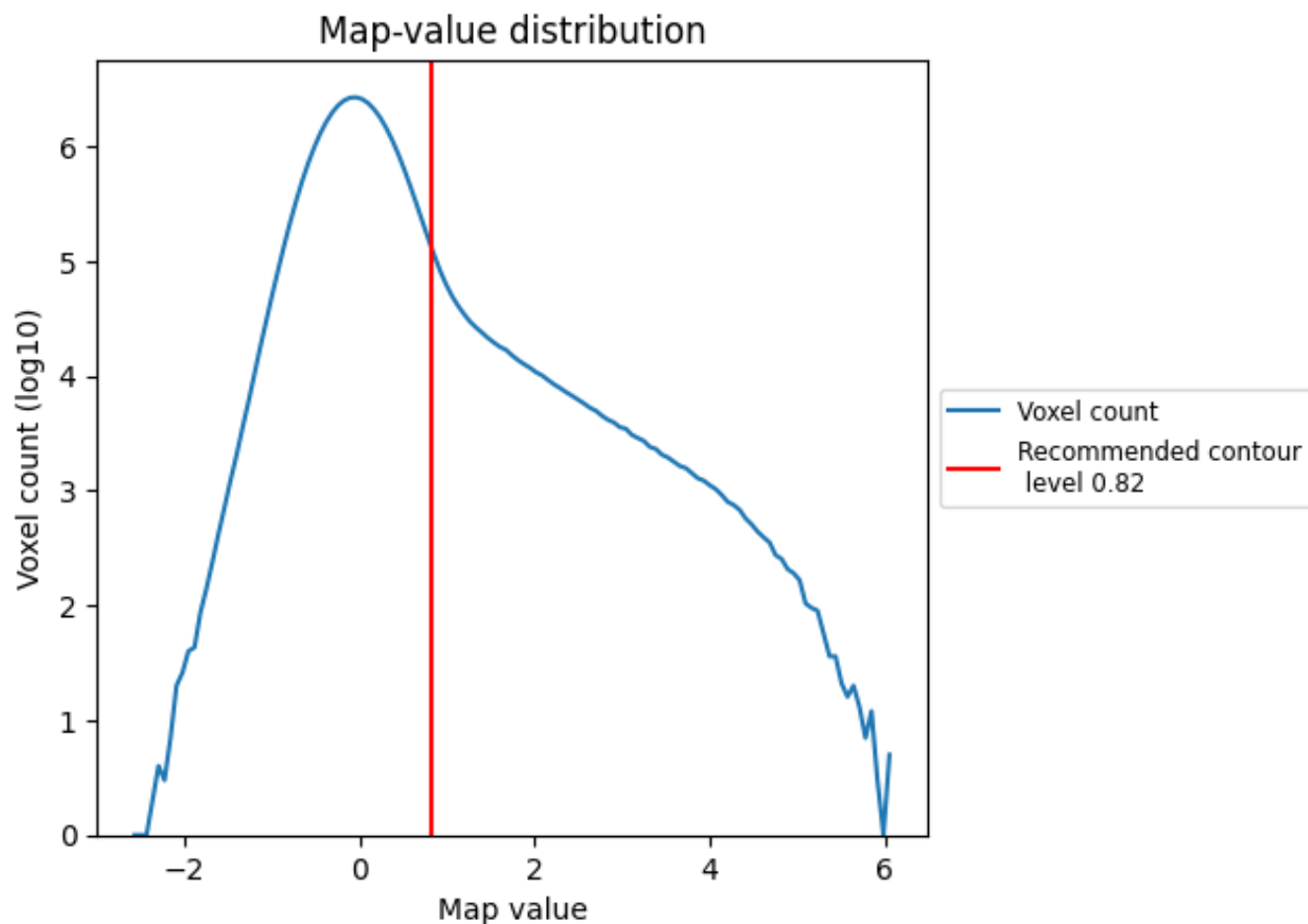
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

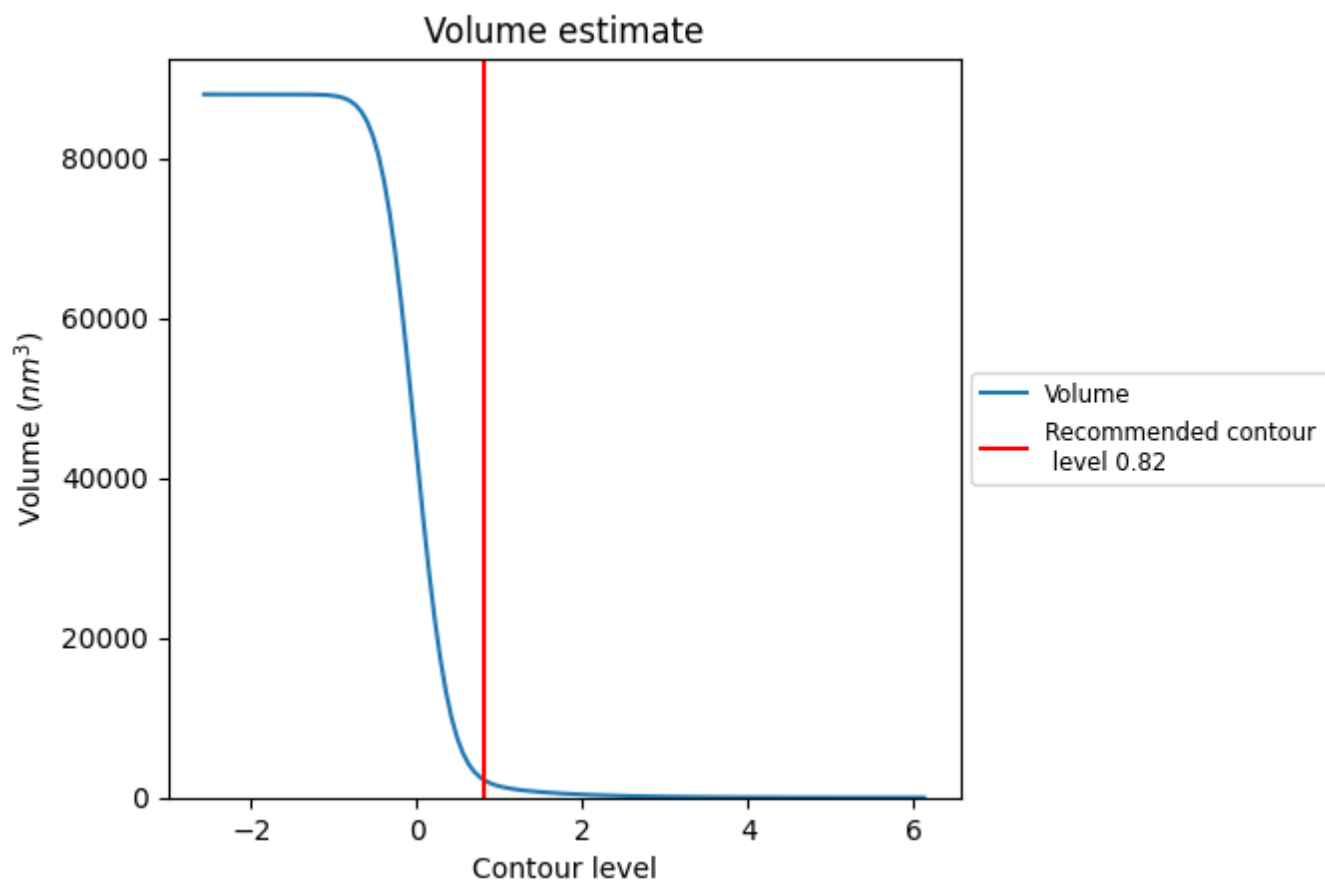
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

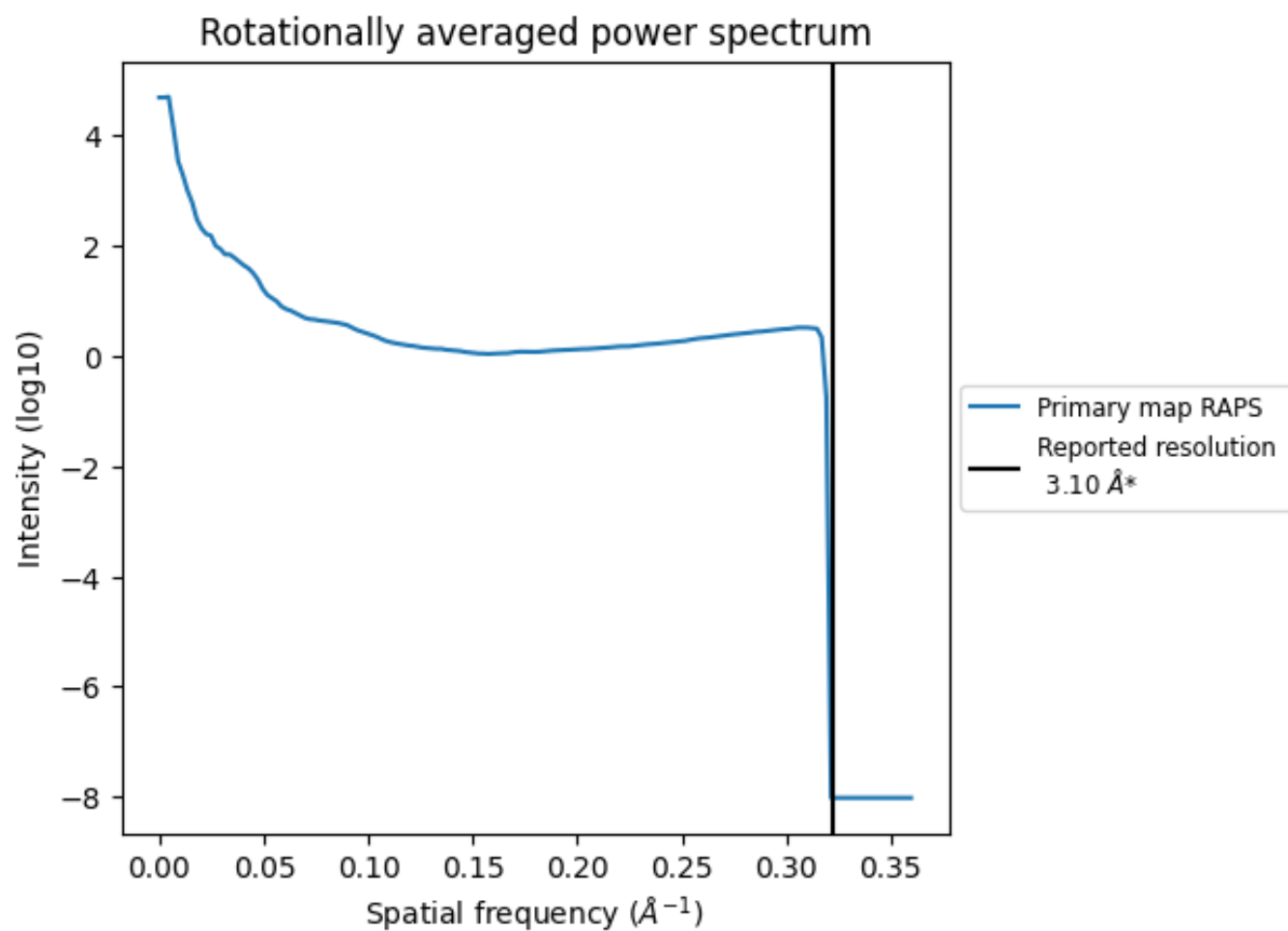
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2156 nm³; this corresponds to an approximate mass of 1948 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 0.323 Å⁻¹

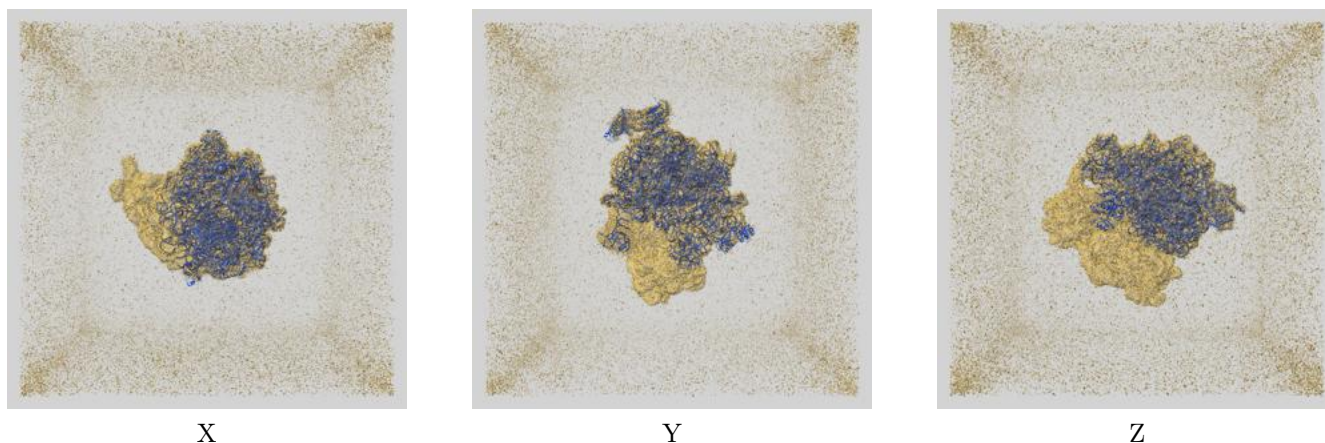
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

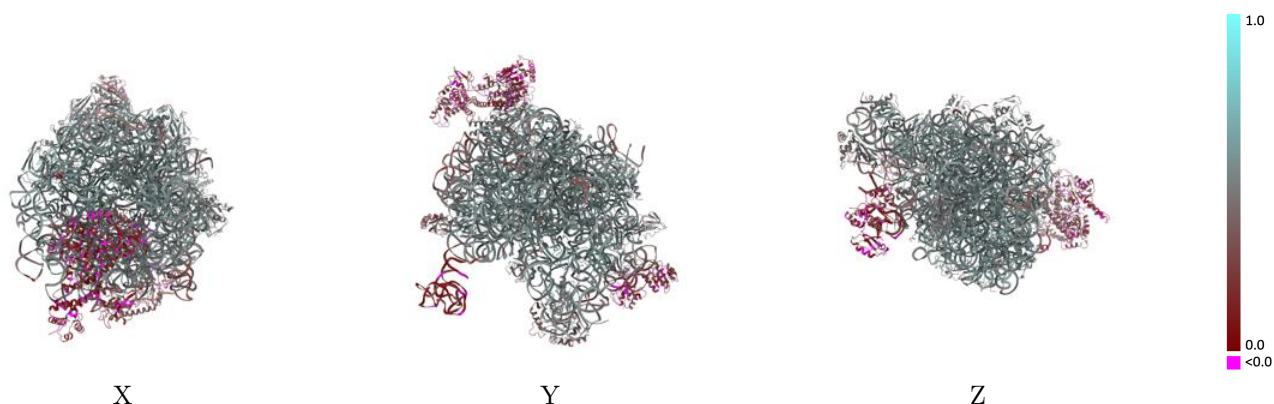
This section contains information regarding the fit between EMDB map EMD-10073 and PDB model 6S0K. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



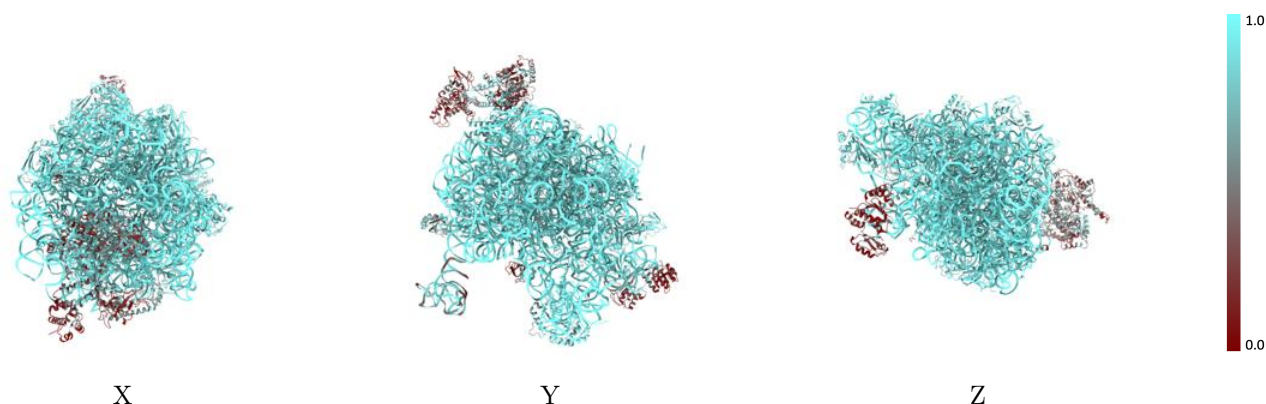
The images above show the 3D surface view of the map at the recommended contour level 0.82 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



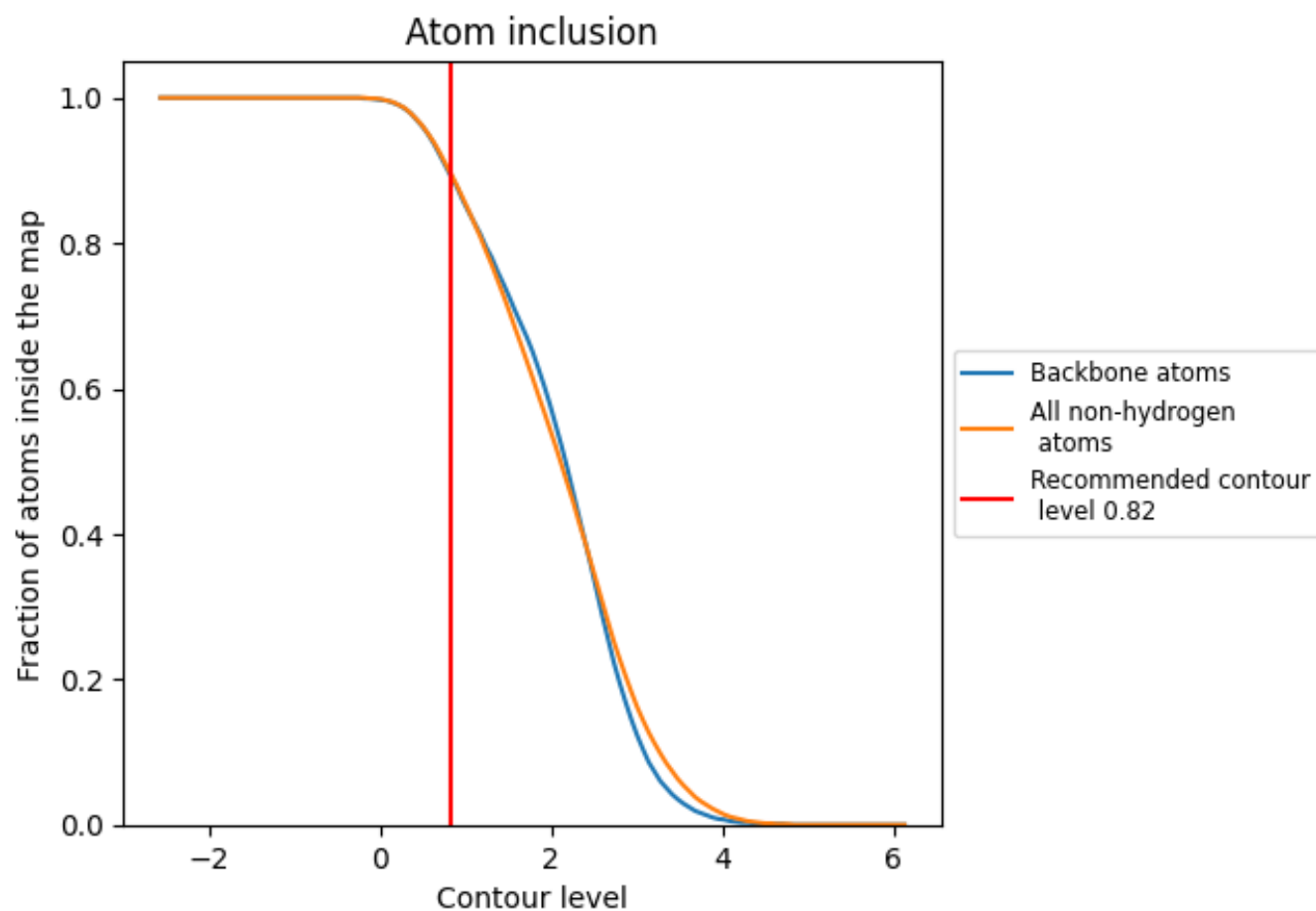
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.82).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 90% 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 (0.82) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8960	 0.4800
2	 0.9190	 0.5050
A	 0.9780	 0.5100
B	 0.9900	 0.4970
C	 0.9230	 0.5540
D	 0.9250	 0.5420
E	 0.9060	 0.5090
F	 0.8530	 0.4200
G	 0.9070	 0.4680
H	 0.5930	 0.3700
I	 0.1720	 0.1650
J	 0.2120	 0.1100
K	 0.9370	 0.5470
L	 0.8840	 0.5390
M	 0.9340	 0.5410
N	 0.9210	 0.5420
O	 0.9210	 0.5330
P	 0.9400	 0.4950
Q	 0.9010	 0.5330
R	 0.9380	 0.5330
S	 0.9250	 0.5250
T	 0.8930	 0.5240
U	 0.8590	 0.5130
V	 0.9150	 0.4960
W	 0.9250	 0.5170
X	 0.9330	 0.5570
Y	 0.9070	 0.5330
Z	 0.8510	 0.4730
a	 0.9110	 0.5310
b	 0.9020	 0.5380
c	 0.2360	 0.4130
d	 0.9180	 0.5580
e	 0.9330	 0.5520
f	 0.9320	 0.5440
h	 0.3510	 0.1690
k	 0.4930	 0.3020

