Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 02:03 am GMT

PDB ID	:	6GC0
EMDB ID	:	EMD-4379
Title	:	50S ribosomal subunit assembly intermediate state 4
Authors	:	Nikolay, R.; Hilal, T.; Qin, B.; Loerke, J.; Buerger, J.; Mielke, T.; Spahn, C.M.T.
Deposited on	:	2018-04-16
Resolution	:	3.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

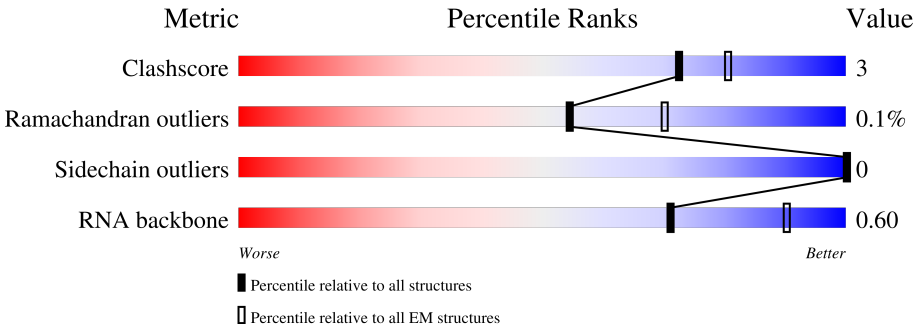
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2904	9% 73% 19% • 6%
2	B	119	• 72% 25% •
3	C	271	7% 80% 20%
4	D	209	17% 87% 13%
5	E	201	16% 89% 11%
6	F	177	40% 87% 13%
7	G	176	94% 93% 7%

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Mol	Chain	Length	Quality of chain
8	H	50	62% 80% 20%
9	J	142	87% 13%
10	K	122	16% 80% 20%
11	L	143	10% 87% 13%
12	N	120	83% 17%
13	O	116	13% 87% 13%
14	P	114	14% 83% 17%
15	Q	117	85% 15%
16	R	103	15% 90% 10%
17	S	110	6% 89% 11%
18	T	93	14% 89% 11%
19	U	102	12% 89% 11%
20	V	94	28% 89% 11%
21	W	76	8% 87% 13%
22	X	77	9% 88% 12%
23	Y	63	41% 94% 6%
24	Z	58	5% 84% 16%
25	0	56	9% 88% 12%
26	1	50	30% 80% 20%
27	2	46	85% 15%
28	3	64	8% 86% 14%

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 84138 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
			Total	C	N	O	P		
1	A	2729	58604	26144	10806	18925	2729	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	119	2548	1135	466	829	118	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	271	2083	1288	423	365	7	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

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

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	177	1411	899	249	257	6	0	0

- Molecule 7 is a protein called 50S ribosomal protein L6.

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

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	50	Total	C	N	O	S	0	0
			384	247	68	68	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

- Molecule 13 is a protein called 50S ribosomal protein L18.

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

- Molecule 14 is a protein called 50S ribosomal protein L19.

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

- Molecule 15 is a protein called 50S ribosomal protein L20.

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

- Molecule 16 is a protein called 50S ribosomal protein L21.

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

- Molecule 17 is a protein called 50S ribosomal protein L22.

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

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	93	Total 739	C 466	N 139	O 132	S 2	0	0

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	U	102	Total 780	C 492	N 146	O 142	0	0

- Molecule 20 is a protein called 50S ribosomal protein L25.

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

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	76	Total	C	N	O	S	0	0
			575	356	117	101	1		

- Molecule 22 is a protein called 50S ribosomal protein L28.

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

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 24 is a protein called 50S ribosomal protein L30.

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

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	1	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 28 is a protein called 50S ribosomal protein L35.

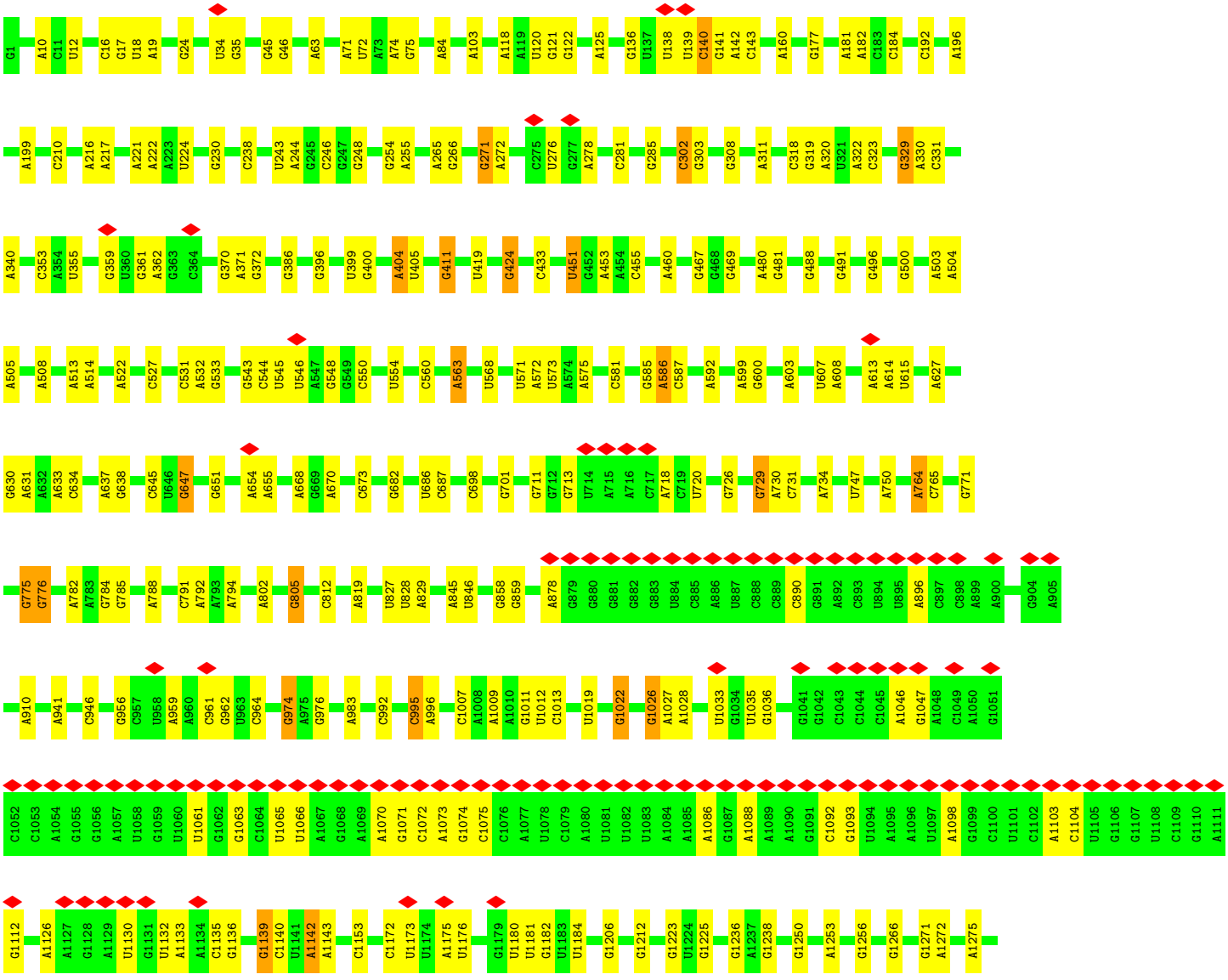
Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

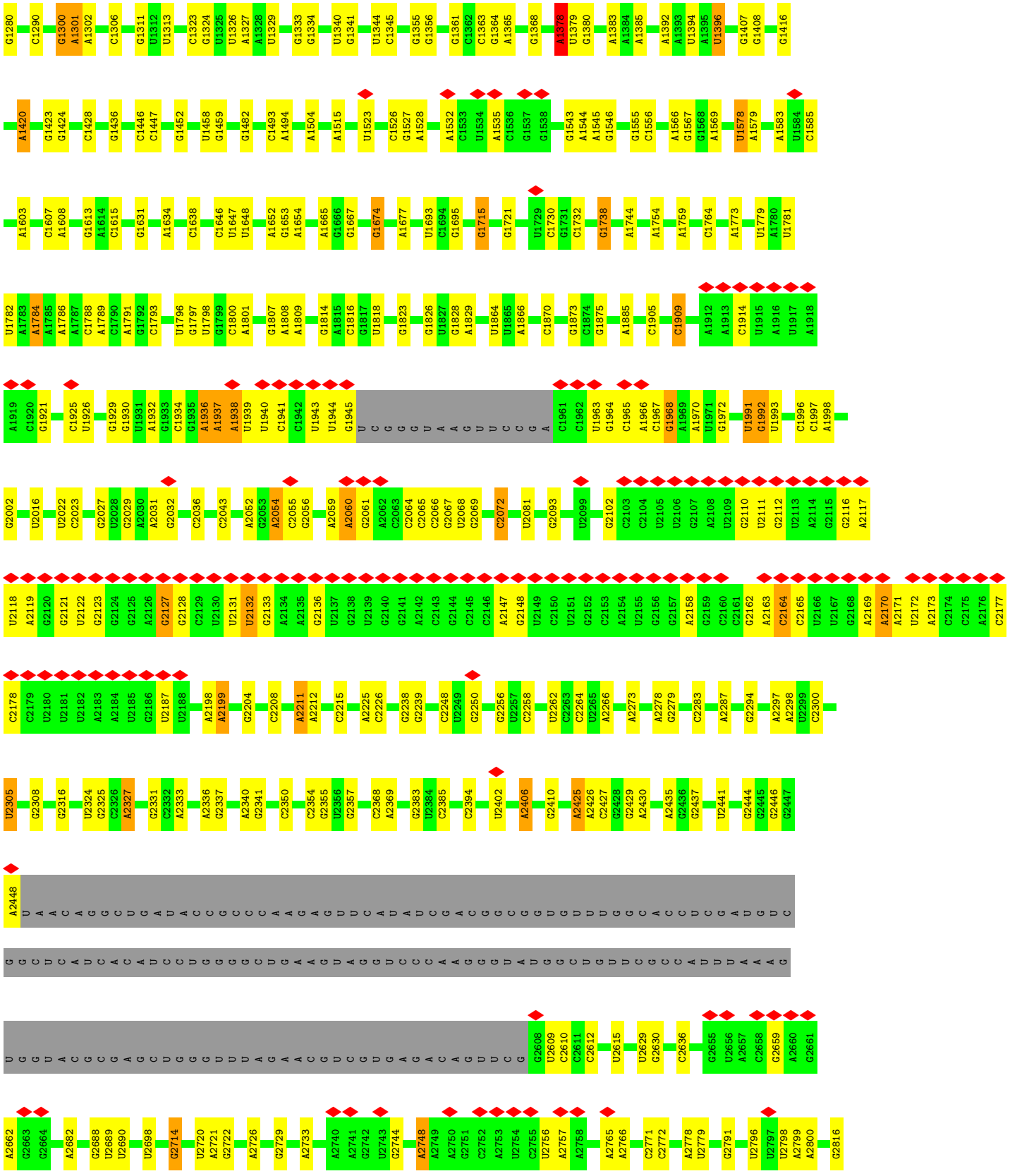
3 Residue-property plots (i)

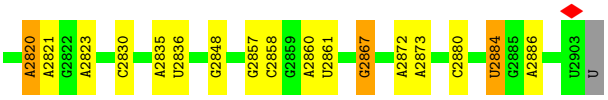
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 23S ribosomal RNA

Chain A: 

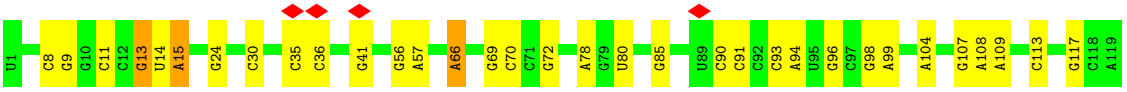



G1280 C1290 G1300 A1301 A1302 C1306 G1311 U1312 U1313 C1323 G1324 U1325 U1326 A1327 A1328 U1329 G1333 G1334 U1340 G1341 U1344 C1345 G1355 G1356 G1361 C1362 C1363 G1364 A1365 G1368 A1378 U1379 G1380 A1383 A1384 A1385 A1392 A1393 U1394 A1395 U1396 G1407 G1408 G1416
A1420 G1423 G1424 C1428 G1436 C1446 C1447 G1452 U1458 G1459 G1482 C1493 A1494 A1504 A1515 U1523 C1526 G1527 A1528 A1532 C1533 U1534 A1535 C1536 G1537 G1538 G1543 A1544 A1545 G1546 G1555 C1556 A1566 G1567 G1568 A1569 U1578 A1579 A1583 U1584 C1585
A1603 C1607 A1608 G1613 A1614 C1615 G1631 A1634 C1638 C1646 U1647 U1648 A1652 G1653 A1654 A1665 G1666 G1667 G1674 A1677 U1693 C1694 G1695 G1715 G1721 U1729 C1730 G1731 C1732 G1738 A1744 A1754 A1759 C1764 A1773 U1779 A1780 U1781
U1782 A1783 A1784 A1785 A1786 A1787 C1788 A1789 C1790 A1791 G1792 C1793 U1796 G1797 U1798 G1799 C1800 A1801 G1807 A1808 A1809 G1814 A1815 C1816 G1817 U1818 G1823 G1826 U1827 G1828 A1829 U1864 U1865 A1866 C1870 G1873 C1874 G1875 A1885 C1905 C1909 A1912 A1913 C1914 U1915 A1916 U1917 A1918
A1919 C1920 G1921 C1925 U1926 G1929 G1930 U1931 A1932 G1933 C1934 G1935 A1936 A1937 A1938 U1939 U1940 C1941 C1942 U1943 U1944 G1945 U C G G G U A A G U U C C G A C1961 C1962 U1963 G1964 C1965 A1966 C1967 G1968 A1969 A1970 U1971 G1972 U1991 G1992 U1993 C1996 C1997 A1998
G2002 U2016 U2022 C2023 G2027 U2028 G2029 A2030 A2031 G2032 C2036 C2043 A2052 G2053 A2054 C2055 G2056 A2059 A2060 G2061 A2062 C2063 C2064 C2065 C2066 G2067 U2068 G2069 C2072 U2081 G2093 U2099 G2102 C2103 C2104 U2105 U2106 G2107 A2108 U2109 G2110 U2111 G2112 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 A2142 C2143 G2144 C2145 C2146 A2147 G2148 U2149 C2150 U2151 G2152 C2153 A2154 U2155 G2156 G2157 A2158 G2159 C2160 C2161 G2162 A2163 C2164 C2165 U2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177
C2178 C2179 U2180 U2181 U2182 A2183 A2184 U2185 G2186 U2187 U2188 A2198 A2199 G2204 C2208 A2211 A2212 C2215 A2225 C2226 G2238 G2239 C2248 U2249 G2250 G2256 U2257 C2258 U2262 C2263 C2264 U2265 A2266 A2273 A2278 G2279 C2283 A2287 G2294 A2297 A2298 U2299 C2300
U2305 G2308 G2316 U2324 G2325 C2326 A2327 G2331 C2332 A2333 A2336 G2337 A2340 G2341 C2350 C2354 G2355 U2356 G2357 C2368 A2369 G2383 U2384 C2385 C2394 U2402 A2406 G2410 A2425 A2426 C2427 G2428 G2429 A2430 A2435 G2436 G2437 U2441 G2444 G2445 G2446 G2447
A2448 U A A C A A G G C U G A U C C C C C G G G A A U C C C C C G G G C C C C U A A A A G C G U U C A A C G A A A A G G U C U C C C C A A G G G G G U C A C C U G G G C U U U G G G C C A A A A C C C C A A A A C C C C U U U U G G G G C C A A A A G G G G U U U U C C C C A A A A G G G G U U U U C C C C A A A A G G G G U U U U C C



• Molecule 2: 5S ribosomal RNA

Chain B:

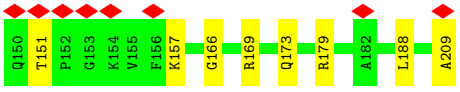


• Molecule 3: 50S ribosomal protein L2

Chain C:

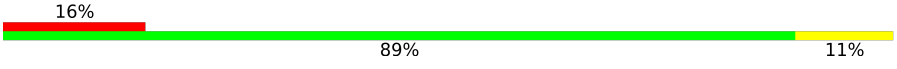
• Molecule 4: 50S ribosomal protein L3

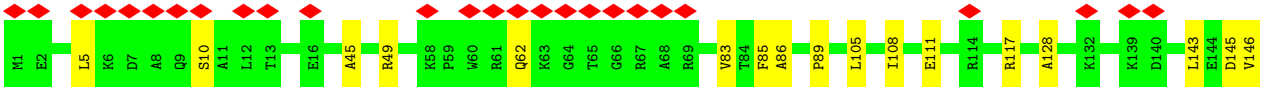
Chain D:

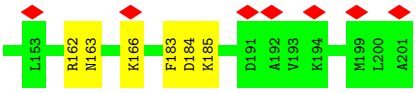


• Molecule 5: 50S ribosomal protein L4

Chain E:

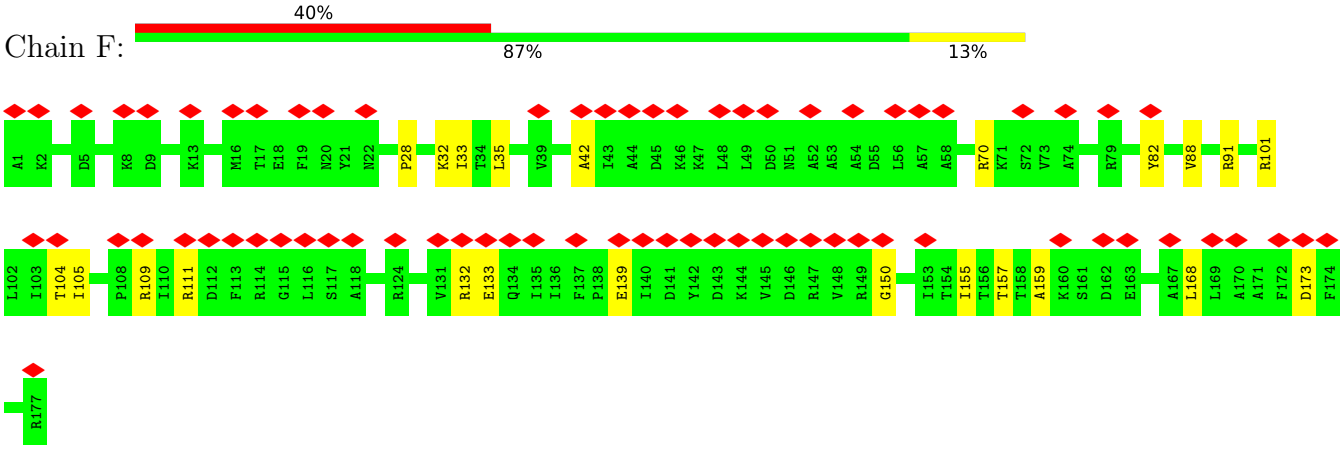






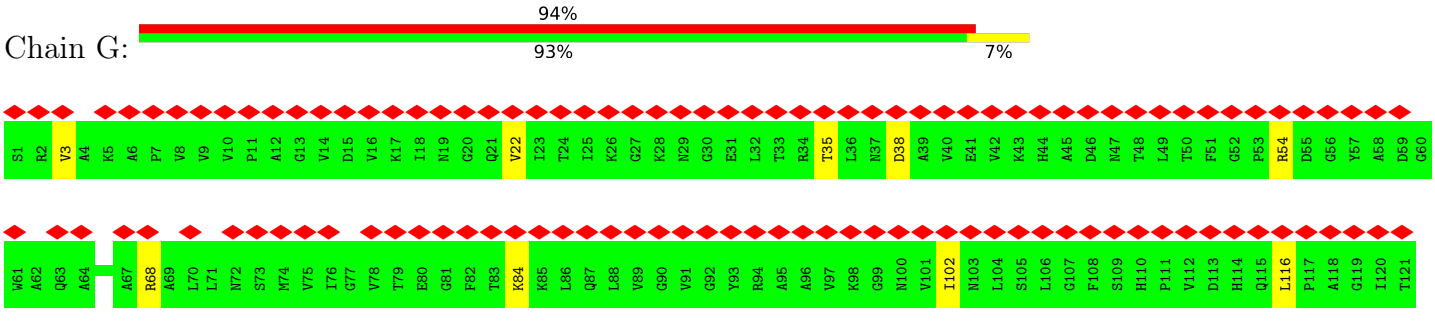
• Molecule 6: 50S ribosomal protein L5

Chain F:



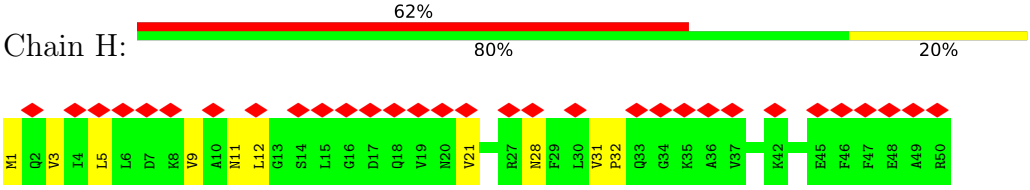
• Molecule 7: 50S ribosomal protein L6

Chain G:



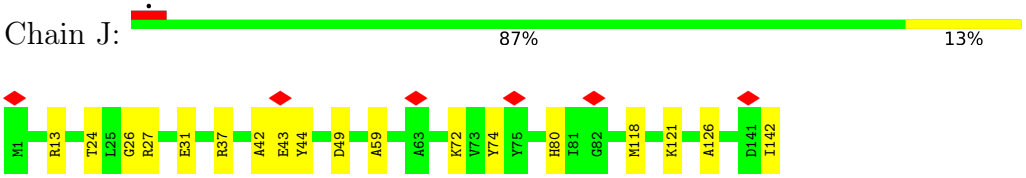
• Molecule 8: 50S ribosomal protein L9

Chain H:



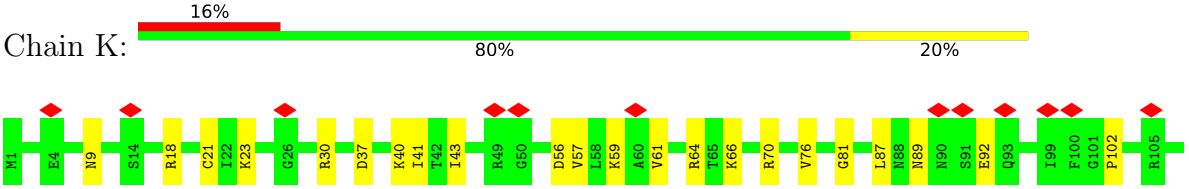
• Molecule 9: 50S ribosomal protein L13

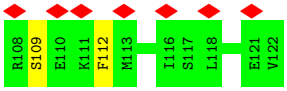
Chain J:



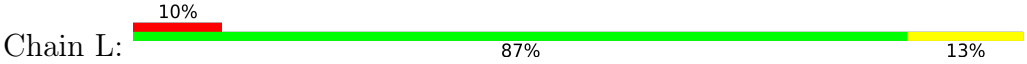
• Molecule 10: 50S ribosomal protein L14

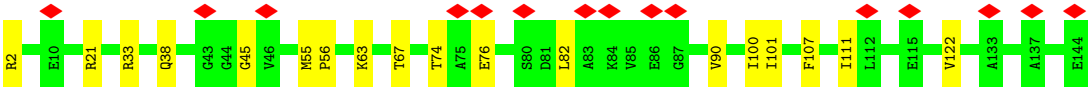
Chain K:



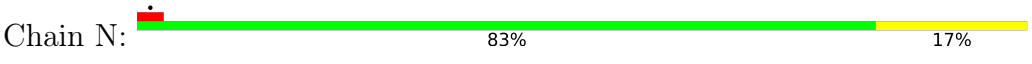


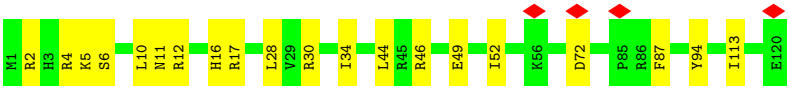
• Molecule 11: 50S ribosomal protein L15



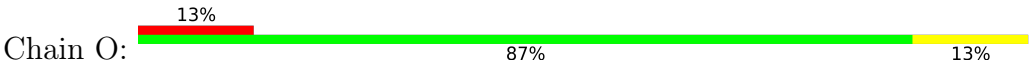


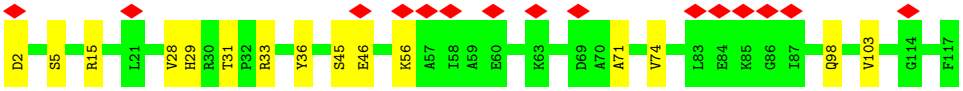
• Molecule 12: 50S ribosomal protein L17



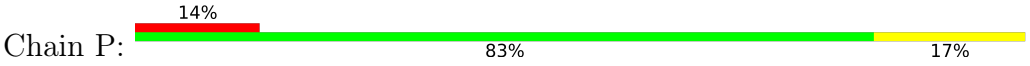


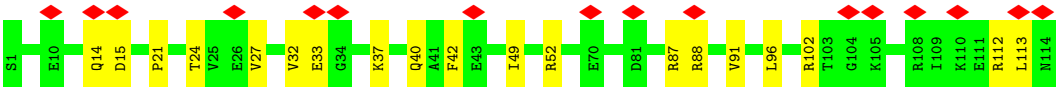
• Molecule 13: 50S ribosomal protein L18



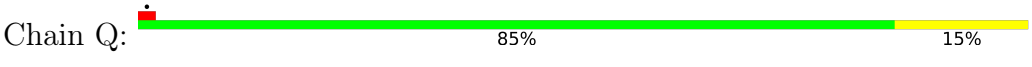


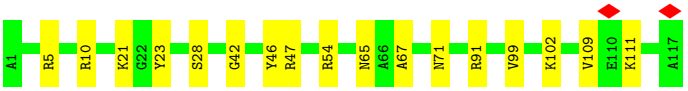
• Molecule 14: 50S ribosomal protein L19



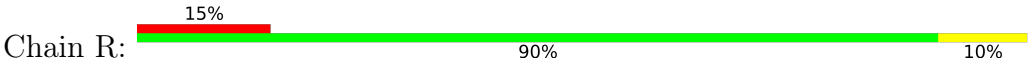


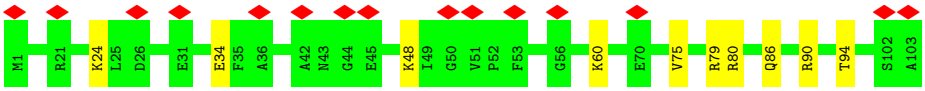
• Molecule 15: 50S ribosomal protein L20





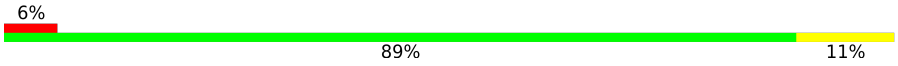
• Molecule 16: 50S ribosomal protein L21





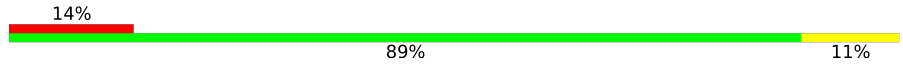
• Molecule 17: 50S ribosomal protein L22

Chain S:



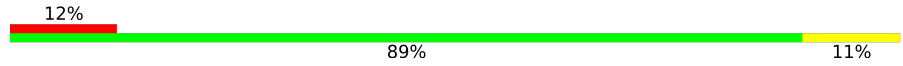
• Molecule 18: 50S ribosomal protein L23

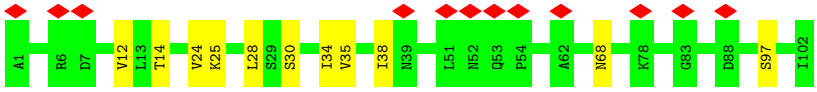
Chain T:



• Molecule 19: 50S ribosomal protein L24

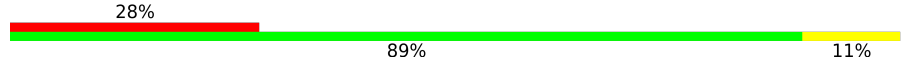
Chain U:

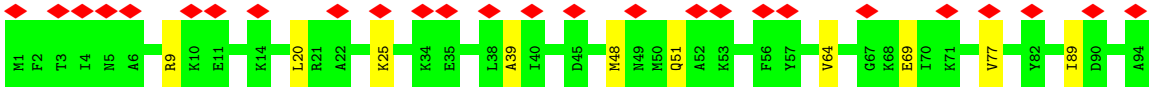




• Molecule 20: 50S ribosomal protein L25

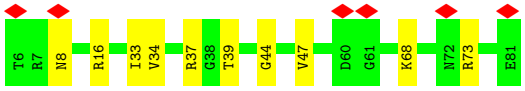
Chain V:





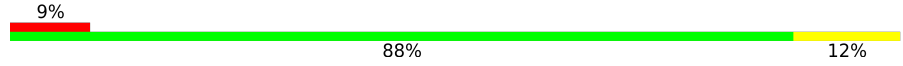
• Molecule 21: 50S ribosomal protein L27

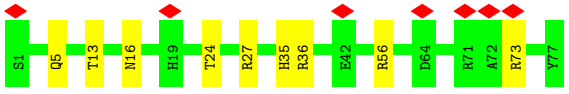
Chain W:



• Molecule 22: 50S ribosomal protein L28

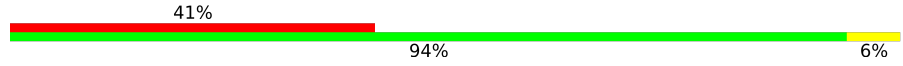
Chain X:

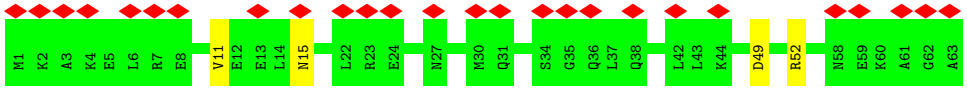




• Molecule 23: 50S ribosomal protein L29

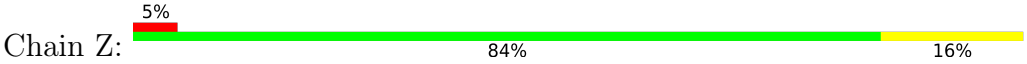
Chain Y:

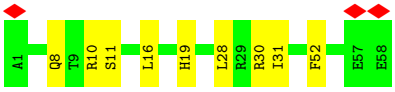




• Molecule 24: 50S ribosomal protein L30

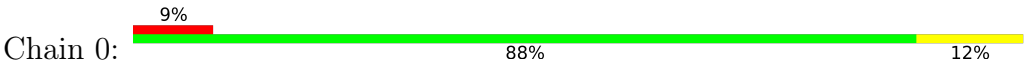
Chain Z:

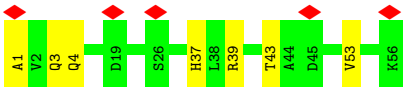




• Molecule 25: 50S ribosomal protein L32

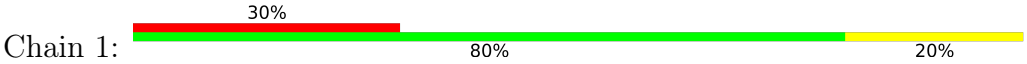
Chain 0:

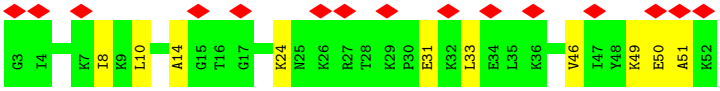




• Molecule 26: 50S ribosomal protein L33

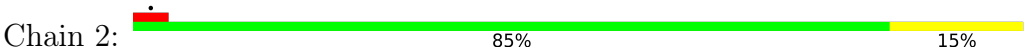
Chain 1:

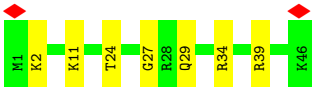




• Molecule 27: 50S ribosomal protein L34

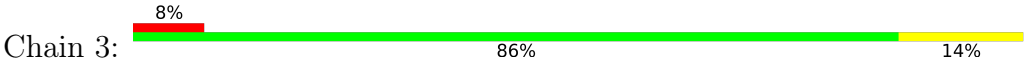
Chain 2:

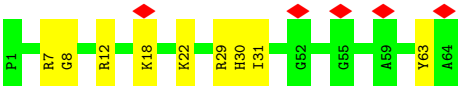




• Molecule 28: 50S ribosomal protein L35

Chain 3:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37815	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	30.860	Depositor
Minimum map value	-16.538	Depositor
Average map value	0.157	Depositor
Map value standard deviation	1.409	Depositor
Recommended contour level	4.5	Depositor
Map size (Å)	334.8, 334.8, 334.8	wwPDB
Map dimensions	270, 270, 270	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.24, 1.24, 1.24	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.18	0/65642	0.77	15/102405 (0.0%)
2	B	0.18	0/2847	0.77	0/4440
3	C	0.26	0/2122	0.54	0/2852
4	D	0.27	0/1586	0.50	0/2134
5	E	0.31	1/1571 (0.1%)	0.47	0/2113
6	F	0.26	0/1435	0.48	0/1926
7	G	0.25	0/1343	0.49	0/1816
8	H	0.29	0/389	0.78	1/523 (0.2%)
9	J	0.24	0/1152	0.45	0/1551
10	K	0.27	0/948	0.54	0/1268
11	L	0.26	0/1054	0.57	1/1403 (0.1%)
12	N	0.26	0/974	0.56	0/1301
13	O	0.24	0/902	0.47	0/1209
14	P	0.27	0/929	0.59	3/1242 (0.2%)
15	Q	0.24	0/960	0.43	0/1278
16	R	0.25	0/829	0.49	0/1107
17	S	0.24	0/864	0.49	0/1156
18	T	0.26	0/745	0.53	0/994
19	U	0.30	0/788	0.61	1/1051 (0.1%)
20	V	0.24	0/766	0.44	0/1025
21	W	0.26	0/582	0.47	0/769
22	X	0.23	0/635	0.45	0/848
23	Y	0.24	0/510	0.46	0/677
24	Z	0.23	0/453	0.46	0/605
25	0	0.23	0/450	0.49	0/599
26	1	0.28	0/417	0.54	0/554
27	2	0.23	0/380	0.43	0/498
28	3	0.27	0/513	0.50	0/676
All	All	0.21	1/91786 (0.0%)	0.72	21/138020 (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
3	C	0	1
4	D	0	1
6	F	0	1
8	H	0	3
10	K	0	1
12	N	0	1
25	0	0	1
28	3	0	1
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	128	ALA	C-N	7.61	1.48	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	P	113	LEU	CA-CB-CG	7.40	132.32	115.30
1	A	2060	A	P-O3'-C3'	7.17	128.31	119.70
14	P	15	ASP	CB-CG-OD1	7.05	124.65	118.30
1	A	1938	A	P-O3'-C3'	6.97	128.07	119.70
1	A	1378	A	P-O3'-C3'	6.69	127.73	119.70
8	H	12	LEU	CA-CB-CG	6.45	130.15	115.30
1	A	271	G	P-O3'-C3'	6.42	127.40	119.70
1	A	545	U	C2-N1-C1'	5.94	124.83	117.70
1	A	2425	A	P-O3'-C3'	5.82	126.68	119.70
1	A	1378	A	OP1-P-O3'	5.77	117.89	105.20
1	A	404	A	P-O3'-C3'	5.69	126.53	119.70
1	A	323	C	N1-C2-O2	5.62	122.28	118.90
11	L	82	LEU	CA-CB-CG	5.60	128.17	115.30
19	U	97	SER	C-N-CA	5.54	135.55	121.70
1	A	995	C	P-O3'-C3'	5.39	126.17	119.70
1	A	2127	G	P-O3'-C3'	5.37	126.14	119.70
1	A	2164	C	N1-C2-O2	5.25	122.05	118.90
1	A	140	C	N1-C2-O2	5.21	122.03	118.90
14	P	14	GLN	C-N-CA	5.17	134.63	121.70
1	A	1313	U	C2-N1-C1'	5.07	123.79	117.70
1	A	974	G	C4-N9-C1'	5.01	133.01	126.50

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	0	53	VAL	Peptide
28	3	30	HIS	Peptide
3	C	11	GLY	Peptide
4	D	151	THR	Peptide
6	F	173	ASP	Peptide
8	H	11	ASN	Peptide
8	H	31	VAL	Peptide
8	H	32	PRO	Peptide
10	K	92	GLU	Peptide
12	N	10	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	58604	0	29475	196	0
2	B	2548	0	1292	16	0
3	C	2083	0	2157	38	0
4	D	1565	0	1616	18	0
5	E	1552	0	1619	15	0
6	F	1411	0	1447	14	0
7	G	1323	0	1374	7	0
8	H	384	0	405	4	0
9	J	1129	0	1162	12	0
10	K	939	0	1012	13	0
11	L	1045	0	1117	13	0
12	N	961	0	1000	12	0
13	O	892	0	923	10	0
14	P	917	0	965	10	0
15	Q	947	0	1022	15	0
16	R	816	0	839	8	0
17	S	857	0	922	8	0
18	T	739	0	807	7	0
19	U	780	0	834	5	0
20	V	753	0	780	5	0
21	W	575	0	589	10	0
22	X	625	0	655	7	0
23	Y	509	0	543	2	0
24	Z	449	0	491	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	0	444	0	461	6	0
26	1	410	0	440	5	0
27	2	377	0	418	5	0
28	3	504	0	574	7	0
All	All	84138	0	54939	379	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 3.

All (379) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:36:ASN:HB2	3:C:61:TYR:HB2	1.75	0.68
1:A:571:U:H2'	16:R:80:ARG:HH12	1.58	0.67
1:A:1652:A:H62	12:N:11:ASN:HD21	1.43	0.67
6:F:35:LEU:HB3	6:F:88:VAL:HB	1.78	0.66
6:F:32:LYS:HD3	6:F:91:ARG:HH11	1.60	0.65
1:A:2394:C:H5"	11:L:63:LYS:HE2	1.78	0.65
1:A:244:A:H5"	11:L:67:THR:HG21	1.78	0.64
1:A:2262:U:H5"	21:W:37:ARG:HH12	1.62	0.64
13:O:29:HIS:HB3	13:O:36:TYR:HB2	1.80	0.63
1:A:585:G:N7	15:Q:5:ARG:NH1	2.47	0.62
1:A:1793:C:H42	1:A:1826:G:H1	1.48	0.62
20:V:20:LEU:HD22	20:V:25:LYS:HD2	1.81	0.62
11:L:90:VAL:HB	11:L:122:VAL:HA	1.82	0.61
12:N:49:GLU:HG2	12:N:94:TYR:HB2	1.83	0.61
1:A:1932:A:H62	1:A:1968:G:H21	1.48	0.61
2:B:30:C:H1'	2:B:57:A:H61	1.66	0.60
1:A:320:A:N3	5:E:163:ASN:ND2	2.50	0.60
1:A:243:U:OP2	28:3:7:ARG:NH2	2.34	0.60
13:O:31:THR:HG22	13:O:33:ARG:H	1.66	0.60
6:F:32:LYS:HB3	6:F:91:ARG:HE	1.66	0.59
10:K:23:LYS:HB2	10:K:40:LYS:HB3	1.85	0.59
21:W:33:ILE:HG22	21:W:34:VAL:HG23	1.83	0.59
1:A:2796:U:H3	1:A:2799:A:H61	1.50	0.59
7:G:84:LYS:HB2	7:G:132:LEU:HB2	1.85	0.59
1:A:687:C:H5"	27:2:2:LYS:HE2	1.85	0.58
3:C:61:TYR:HA	3:C:85:ASN:HD21	1.69	0.58
1:A:1280:G:H1	1:A:1290:C:H42	1.52	0.58
3:C:134:ILE:O	3:C:166:ARG:NH1	2.37	0.58
11:L:76:GLU:HG3	11:L:111:ILE:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:48:MET:SD	20:V:51:GLN:NE2	2.77	0.58
4:D:179:ARG:HB3	4:D:188:LEU:HD12	1.86	0.57
10:K:43:ILE:HD12	10:K:56:ASP:HB2	1.84	0.57
9:J:43:GLU:HG3	15:Q:99:VAL:HG13	1.86	0.57
1:A:1866:A:H62	1:A:1875:G:H21	1.52	0.57
2:B:11:C:OP1	21:W:68:LYS:NZ	2.34	0.57
1:A:19:A:H5"	15:Q:21:LYS:HE2	1.86	0.57
14:P:91:VAL:HG21	14:P:96:LEU:HD21	1.86	0.57
1:A:713:G:H21	1:A:718:A:H62	1.53	0.56
1:A:1789:A:OP2	3:C:220:ARG:NH1	2.38	0.56
11:L:74:THR:HG22	11:L:107:PHE:HB2	1.86	0.56
27:2:24:THR:HG23	27:2:27:GLY:H	1.70	0.56
1:A:1674:G:N2	1:A:1677:A:N1	2.53	0.56
1:A:281:C:H42	1:A:359:G:H1	1.53	0.56
15:Q:23:TYR:H	15:Q:28:SER:HB3	1.70	0.56
1:A:1526:C:H42	1:A:1546:G:H1	1.51	0.56
3:C:149:LYS:HE2	3:C:152:GLN:HE22	1.71	0.56
1:A:1909:C:H42	1:A:1921:G:H1	1.53	0.56
1:A:246:C:H41	28:3:7:ARG:HG2	1.71	0.55
18:T:59:ASN:HB2	18:T:84:TYR:HB2	1.88	0.55
17:S:59:GLU:HA	17:S:64:ALA:HB2	1.88	0.55
18:T:6:ARG:NH2	18:T:37:ASP:OD2	2.40	0.55
3:C:143:VAL:HB	3:C:153:LEU:HB2	1.89	0.55
1:A:1364:G:H5'	1:A:1809:A:H1'	1.89	0.54
1:A:1759:A:HO2'	1:A:2714:G:HO2'	1.54	0.54
1:A:1788:C:OP1	3:C:220:ARG:NH2	2.41	0.54
5:E:146:VAL:HG12	5:E:185:LYS:HB2	1.90	0.54
1:A:1779:U:OP2	1:A:1784:A:N6	2.41	0.54
1:A:1992:G:N2	1:A:1996:C:O2'	2.41	0.54
1:A:2659:G:N2	1:A:2662:A:OP2	2.39	0.54
8:H:1:MET:N	8:H:21:VAL:O	2.40	0.54
23:Y:49:ASP:OD1	23:Y:52:ARG:NH2	2.40	0.54
26:1:14:ALA:HB2	26:1:46:VAL:HG21	1.89	0.54
1:A:500:G:N1	1:A:503:A:OP2	2.41	0.54
1:A:2720:U:OP1	14:P:52:ARG:NH2	2.34	0.54
10:K:30:ARG:NH2	10:K:37:ASP:OD2	2.41	0.54
1:A:1311:G:H21	1:A:1603:A:H62	1.56	0.53
3:C:106:PRO:HD2	3:C:109:LEU:HD22	1.90	0.53
17:S:9:HIS:O	17:S:11:ARG:NH1	2.42	0.53
1:A:2444:G:OP1	5:E:62:GLN:NE2	2.41	0.53
10:K:66:LYS:HD3	10:K:81:GLY:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:5:LEU:HD22	8:H:9:VAL:HG21	1.90	0.53
1:A:2131:U:H5'	1:A:2132:U:H5"	1.90	0.53
1:A:2688:G:N1	1:A:2720:U:OP2	2.35	0.53
4:D:7:LYS:HD2	4:D:77:ARG:HH22	1.74	0.53
15:Q:111:LYS:HG3	16:R:48:LYS:HD2	1.91	0.53
19:U:28:LEU:HD12	19:U:30:SER:H	1.74	0.53
1:A:1791:A:N6	1:A:1828:G:O2'	2.40	0.53
3:C:10:PRO:HA	3:C:13:ARG:HB2	1.91	0.53
1:A:2054:A:O2'	25:0:4:GLN:NE2	2.41	0.53
1:A:2002:G:OP1	12:N:17:ARG:NH2	2.41	0.53
1:A:2357:G:OP1	21:W:16:ARG:NH1	2.42	0.53
1:A:729:G:N2	3:C:10:PRO:O	2.42	0.52
1:A:2248:C:H42	1:A:2256:G:H1	1.56	0.52
1:A:2199:A:OP1	22:X:36:ARG:NH1	2.43	0.52
4:D:53:GLY:HA3	4:D:77:ARG:HE	1.74	0.52
3:C:144:GLU:HB3	3:C:187:CYS:HB3	1.91	0.52
1:A:1022:G:N2	1:A:1142:A:N1	2.57	0.52
14:P:27:VAL:HB	14:P:42:PHE:HB3	1.92	0.52
1:A:2081:U:H4'	22:X:24:THR:HG21	1.92	0.52
1:A:1818:U:H2'	3:C:155:ARG:HG2	1.91	0.52
1:A:587:C:OP1	11:L:21:ARG:NH1	2.42	0.52
1:A:527:C:N4	1:A:2779:U:OP2	2.41	0.51
1:A:1153:C:OP1	15:Q:91:ARG:NH2	2.42	0.51
4:D:157:LYS:HB2	9:J:80:HIS:HA	1.92	0.51
12:N:28:LEU:HD13	12:N:34:ILE:HG12	1.91	0.51
1:A:2027:G:H1	1:A:2036:C:H42	1.57	0.51
6:F:157:THR:HG22	6:F:159:ALA:H	1.75	0.51
9:J:31:GLU:HG2	9:J:142:ILE:HG12	1.93	0.51
1:A:764:A:N3	3:C:211:ARG:NH2	2.58	0.51
3:C:77:VAL:HG21	3:C:109:LEU:HD11	1.92	0.51
5:E:117:ARG:NH2	5:E:183:PHE:O	2.44	0.51
1:A:24:G:N2	17:S:78:GLU:OE2	2.43	0.51
1:A:2771:C:O2'	4:D:173:GLN:NE2	2.41	0.51
5:E:83:VAL:HB	5:E:86:ALA:HB2	1.93	0.51
3:C:106:PRO:HG2	3:C:109:LEU:HB2	1.92	0.51
3:C:261:ARG:O	3:C:264:LYS:NZ	2.43	0.51
3:C:7:PRO:HB3	3:C:13:ARG:HG3	1.93	0.51
1:A:513:A:O2'	15:Q:10:ARG:NH2	2.45	0.51
1:A:2278:A:H5"	21:W:8:ASN:HD21	1.75	0.51
4:D:136:ASN:OD1	4:D:139:SER:OG	2.28	0.51
1:A:2054:A:N3	25:0:4:GLN:NE2	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:163:ILE:HG12	3:C:173:LEU:HG	1.93	0.50
11:L:63:LYS:O	28:3:29:ARG:NH1	2.44	0.50
1:A:1011:G:OP2	15:Q:65:ASN:ND2	2.44	0.50
1:A:18:U:H3	1:A:522:A:H61	1.60	0.50
1:A:1796:U:H3	1:A:1823:G:H1	1.59	0.50
2:B:78:A:H62	2:B:98:G:H21	1.59	0.50
9:J:59:ALA:H	9:J:126:ALA:HA	1.77	0.50
10:K:40:LYS:HE2	10:K:57:VAL:HG12	1.94	0.50
12:N:44:LEU:HD23	12:N:113:ILE:HD13	1.93	0.50
1:A:1361:G:HO2'	1:A:2215:C:HO2'	1.60	0.50
26:1:8:ILE:HB	26:1:51:ALA:HB1	1.94	0.50
1:A:210:C:OP1	27:2:29:GLN:NE2	2.45	0.50
1:A:668:A:H2'	1:A:670:A:H62	1.77	0.50
1:A:750:A:OP1	1:A:1615:C:N4	2.43	0.50
10:K:59:LYS:NZ	10:K:89:ASN:OD1	2.42	0.50
11:L:38:GLN:NE2	11:L:45:GLY:O	2.45	0.49
3:C:71:ASP:OD2	3:C:188:ARG:NH1	2.45	0.49
6:F:28:PRO:HB2	6:F:168:LEU:HD22	1.94	0.49
23:Y:11:VAL:O	23:Y:15:ASN:ND2	2.45	0.49
1:A:964:C:O2'	1:A:2273:A:N3	2.41	0.49
1:A:805:G:H5"	11:L:38:GLN:HG3	1.94	0.49
1:A:2266:A:N6	1:A:2273:A:OP2	2.46	0.49
14:P:88:ARG:HD2	14:P:112:ARG:HH22	1.78	0.49
1:A:956:G:O2'	1:A:959:A:N6	2.45	0.49
1:A:592:A:HO2'	28:3:63:TYR:HH	1.60	0.49
3:C:166:ARG:HA	3:C:171:VAL:HG12	1.94	0.49
5:E:111:GLU:HG2	11:L:2:ARG:HH21	1.78	0.49
1:A:682:G:O6	1:A:794:A:N6	2.45	0.49
1:A:788:A:OP1	1:A:791:C:N4	2.42	0.49
3:C:130:PRO:HG3	3:C:188:ARG:HG2	1.95	0.49
17:S:73:LYS:HB2	17:S:106:VAL:HB	1.95	0.49
1:A:1527:G:H21	1:A:1545:A:H62	1.61	0.49
1:A:2820:A:OP2	1:A:2821:A:N6	2.45	0.49
10:K:64:ARG:NH1	10:K:102:PRO:O	2.43	0.49
17:S:24:ILE:HD13	17:S:36:LEU:HD11	1.95	0.49
1:A:976:G:O2'	15:Q:54:ARG:NH2	2.45	0.48
9:J:13:ARG:NH1	9:J:49:ASP:O	2.46	0.48
10:K:9:ASN:OD1	10:K:18:ARG:NH1	2.46	0.48
14:P:33:GLU:OE2	14:P:40:GLN:NE2	2.46	0.48
24:Z:10:ARG:NH2	24:Z:52:PHE:O	2.46	0.48
1:A:1754:A:O3'	14:P:102:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2333:A:OP2	21:W:73:ARG:NH2	2.46	0.48
1:A:182:A:N3	1:A:433:C:O2'	2.44	0.48
1:A:411:G:OP2	1:A:2406:A:O2'	2.31	0.48
3:C:170:TYR:HA	3:C:184:GLU:HA	1.94	0.48
20:V:77:VAL:HG23	20:V:89:ILE:HG12	1.94	0.48
1:A:2300:C:H42	1:A:2316:G:H1	1.61	0.48
2:B:66:A:OP2	2:B:108:A:N6	2.46	0.48
1:A:1275:A:OP2	1:A:1646:C:N4	2.47	0.48
1:A:1631:G:N2	1:A:1634:A:OP2	2.43	0.48
12:N:30:ARG:NH2	12:N:72:ASP:OD2	2.47	0.48
1:A:962:G:O2'	1:A:2250:G:N2	2.46	0.48
1:A:2258:C:O2'	1:A:2427:C:OP2	2.32	0.48
17:S:69:LEU:HA	17:S:109:ASP:HA	1.96	0.48
1:A:2262:U:OP1	21:W:37:ARG:NH2	2.46	0.48
1:A:2721:A:OP1	14:P:52:ARG:NE	2.47	0.48
1:A:2748:A:H5'	7:G:3:VAL:HG21	1.94	0.48
1:A:775:G:H4'	1:A:776:G:H5'	1.96	0.47
1:A:2772:C:H5'	4:D:173:GLN:HE21	1.78	0.47
1:A:2884:U:OP2	25:0:39:ARG:NH2	2.47	0.47
10:K:109:SER:HB2	10:K:112:PHE:HD2	1.78	0.47
1:A:460:A:H62	1:A:469:G:H21	1.62	0.47
1:A:1407:G:H2'	1:A:1408:G:H8	1.79	0.47
1:A:2072:C:H42	1:A:2437:G:H1	1.60	0.47
3:C:226:PRO:HB3	3:C:232:GLY:HA2	1.97	0.47
7:G:38:ASP:OD1	7:G:54:ARG:NH1	2.48	0.47
1:A:1798:U:H5"	3:C:257:ARG:HB2	1.97	0.47
9:J:72:LYS:HE3	9:J:74:TYR:HE1	1.80	0.47
12:N:6:SER:HB3	12:N:46:ARG:HH12	1.79	0.47
17:S:9:HIS:HB3	17:S:11:ARG:HH12	1.80	0.47
22:X:5:GLN:O	22:X:73:ARG:NH1	2.47	0.47
1:A:1028:A:OP2	1:A:1126:A:N6	2.41	0.47
1:A:1323:C:N4	1:A:1324:G:O6	2.48	0.47
1:A:1936:A:H2'	1:A:1937:A:H4'	1.97	0.47
1:A:2279:G:HO2'	1:A:2327:A:HO2'	1.62	0.47
1:A:177:G:OP2	1:A:177:G:N2	2.43	0.47
1:A:2857:G:N2	1:A:2860:A:OP2	2.40	0.47
3:C:180:MET:SD	3:C:268:ARG:NH2	2.88	0.47
13:O:2:ASP:HB3	13:O:5:SER:HB2	1.97	0.47
1:A:651:G:H5'	28:3:18:LYS:HG3	1.96	0.46
1:A:673:C:OP1	5:E:49:ARG:NH2	2.46	0.46
1:A:1394:U:H4'	1:A:1603:A:H4'	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:G:H1	1:A:720:U:H3	1.63	0.46
1:A:2336:A:H61	21:W:39:THR:HG21	1.81	0.46
1:A:2612:C:O2	25:0:1:ALA:N	2.49	0.46
4:D:115:GLY:HA2	4:D:166:GLY:HA3	1.97	0.46
6:F:104:THR:HG23	6:F:105:ILE:HG23	1.98	0.46
1:A:698:C:O2'	1:A:734:A:N6	2.49	0.46
1:A:1378:A:O2'	1:A:1380:G:OP2	2.33	0.46
1:A:1436:G:H1	1:A:1556:C:H42	1.63	0.46
10:K:21:CYS:HA	10:K:41:ILE:HG22	1.96	0.46
26:1:10:LEU:HD21	26:1:33:LEU:HD23	1.97	0.46
1:A:1665:A:H5"	10:K:66:LYS:HG3	1.97	0.46
1:A:2163:A:OP1	1:A:2170:A:O2'	2.32	0.46
16:R:34:GLU:HG2	16:R:60:LYS:HG2	1.97	0.46
26:1:24:LYS:NZ	26:1:31:GLU:O	2.45	0.46
1:A:192:C:O2'	1:A:802:A:N3	2.46	0.46
3:C:52:HIS:HA	3:C:216:ARG:HB2	1.96	0.46
4:D:106:LYS:NZ	4:D:209:ALA:OXT	2.45	0.46
6:F:111:ARG:NH2	6:F:133:GLU:OE1	2.42	0.46
1:A:1528:A:N6	1:A:1543:G:O2'	2.49	0.46
1:A:2340:A:H2'	1:A:2341:G:H8	1.81	0.46
7:G:22:VAL:HG12	7:G:35:THR:HG22	1.98	0.46
24:Z:11:SER:HB2	24:Z:31:ILE:HD11	1.98	0.46
1:A:587:C:N3	11:L:33:ARG:NH2	2.63	0.46
1:A:1086:A:H1'	1:A:1103:A:H61	1.79	0.46
1:A:1326:U:H2'	1:A:1327:A:H8	1.81	0.46
1:A:1653:G:N1	12:N:11:ASN:OD1	2.48	0.45
3:C:70:LYS:O	3:C:117:SER:OG	2.30	0.45
1:A:340:A:H4'	5:E:162:ARG:HH12	1.81	0.45
1:A:2305:U:C2	6:F:150:GLY:HA3	2.51	0.45
4:D:121:THR:HG21	4:D:143:PRO:HG3	1.98	0.45
1:A:771:G:OP2	27:2:11:LYS:NZ	2.49	0.45
9:J:37:ARG:NE	9:J:44:TYR:OH	2.50	0.45
1:A:1300:G:H4'	1:A:1301:A:H5"	1.97	0.45
13:O:71:ALA:HA	13:O:74:VAL:HG12	1.99	0.45
28:3:8:GLY:O	28:3:12:ARG:NH2	2.46	0.45
1:A:1998:A:OP2	4:D:141:ARG:NH1	2.50	0.45
1:A:160:A:N3	1:A:2208:C:O2'	2.45	0.45
2:B:13:G:O2'	2:B:15:A:OP2	2.31	0.45
2:B:8:C:H5"	13:O:15:ARG:HH12	1.81	0.45
2:B:72:G:H21	2:B:104:A:H62	1.64	0.45
1:A:184:C:O2'	1:A:217:A:N3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2298:A:OP1	6:F:70:ARG:NH2	2.44	0.45
5:E:117:ARG:NE	5:E:184:ASP:O	2.42	0.45
9:J:42:ALA:HB2	15:Q:67:ALA:HB2	1.99	0.45
1:A:1007:C:OP1	9:J:37:ARG:NH2	2.50	0.45
12:N:52:ILE:HG21	12:N:87:PHE:HD2	1.82	0.45
19:U:24:VAL:HG22	19:U:35:VAL:HG22	1.98	0.45
1:A:1340:U:OP1	18:T:84:TYR:OH	2.33	0.44
5:E:5:LEU:HD22	5:E:10:SER:HB3	1.98	0.44
24:Z:16:LEU:HB2	24:Z:19:HIS:HD2	1.83	0.44
1:A:1385:A:O2'	1:A:1396:U:O2	2.32	0.44
1:A:1392:A:N6	18:T:18:GLU:OE2	2.49	0.44
5:E:105:LEU:HA	5:E:108:ILE:HG22	1.99	0.44
1:A:1184:U:OP2	24:Z:30:ARG:NH2	2.50	0.44
1:A:308:G:H21	1:A:329:G:H21	1.65	0.44
1:A:451:U:O2	1:A:453:A:N6	2.50	0.44
1:A:1363:C:O2'	1:A:1809:A:N3	2.41	0.44
5:E:143:LEU:HD13	5:E:146:VAL:HG11	1.99	0.44
19:U:12:VAL:HG21	19:U:38:ILE:HG21	2.00	0.44
24:Z:8:GLN:HB2	24:Z:28:LEU:HD13	1.99	0.44
1:A:630:G:N2	1:A:633:A:OP2	2.38	0.44
18:T:28:ASN:OD1	18:T:91:GLN:NE2	2.49	0.44
1:A:1721:G:H2'	1:A:1738:G:H22	1.83	0.44
2:B:9:G:H1'	13:O:45:SER:HA	2.00	0.44
10:K:61:VAL:HB	10:K:87:LEU:HD11	1.98	0.44
2:B:14:U:OP2	2:B:70:C:O2'	2.31	0.44
1:A:992:C:OP1	15:Q:46:TYR:OH	2.34	0.44
1:A:1223:G:OP2	16:R:90:ARG:NH1	2.50	0.44
1:A:2848:G:O2'	1:A:2867:G:N2	2.41	0.44
3:C:152:GLN:HA	3:C:155:ARG:HH21	1.81	0.44
3:C:244:VAL:HG12	3:C:250:GLN:HA	1.99	0.44
6:F:42:ALA:O	6:F:82:TYR:OH	2.36	0.44
1:A:1864:U:OP1	1:A:2410:G:O2'	2.34	0.43
5:E:145:ASP:HB2	5:E:166:LYS:HD3	2.00	0.43
1:A:630:G:OP2	28:3:22:LYS:NZ	2.46	0.43
1:A:2636:C:HO2'	4:D:45:TYR:HH	1.65	0.43
14:P:24:THR:HB	14:P:87:ARG:HB3	2.00	0.43
1:A:1035:U:H2'	1:A:1036:G:H8	1.82	0.43
5:E:45:ALA:HB2	5:E:89:PRO:HD3	1.99	0.43
11:L:100:ILE:HG23	11:L:101:ILE:HG23	2.00	0.43
20:V:64:VAL:HG22	20:V:69:GLU:HB3	1.99	0.43
1:A:572:A:H61	1:A:2029:G:H21	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:33:ILE:HG12	6:F:155:ILE:HG13	1.99	0.43
1:A:2354:C:H2'	1:A:2355:G:H8	1.84	0.43
22:X:16:ASN:HB2	22:X:24:THR:HB	2.01	0.43
3:C:158:GLY:O	3:C:176:ARG:NH2	2.52	0.43
7:G:126:THR:HB	7:G:129:GLU:HB2	2.01	0.43
13:O:28:VAL:HG11	13:O:103:VAL:HG13	2.01	0.43
1:A:1225:G:O3'	16:R:86:GLN:NE2	2.51	0.43
1:A:1693:U:O2	3:C:13:ARG:NH2	2.51	0.43
15:Q:99:VAL:O	15:Q:102:LYS:NZ	2.52	0.43
1:A:370:G:O2'	1:A:424:G:OP1	2.36	0.43
1:A:607:U:H2'	1:A:608:A:H8	1.83	0.43
1:A:1019:U:H3	1:A:1142:A:H62	1.65	0.43
1:A:1814:G:OP1	3:C:39:SER:OG	2.36	0.43
1:A:2066:C:N4	1:A:2067:G:O6	2.51	0.43
1:A:2368:C:H2'	1:A:2369:A:H8	1.84	0.43
2:B:13:G:H1	2:B:69:G:HO2'	1.67	0.43
2:B:93:C:H2'	2:B:94:A:H8	1.84	0.43
8:H:1:MET:HG3	8:H:3:VAL:HG13	2.01	0.43
1:A:1139:G:O2'	1:A:1143:A:N1	2.44	0.42
2:B:113:C:H1'	13:O:46:GLU:HA	2.01	0.42
1:A:1638:C:O2	1:A:2698:U:O2'	2.34	0.42
27:2:34:ARG:HD2	27:2:39:ARG:HD2	2.01	0.42
2:B:85:G:H1	2:B:91:C:H42	1.67	0.42
19:U:14:THR:OG1	19:U:68:ASN:ND2	2.52	0.42
1:A:285:G:H1	1:A:355:U:H3	1.68	0.42
1:A:599:A:H2'	1:A:600:G:H8	1.83	0.42
4:D:131:ASP:O	4:D:136:ASN:ND2	2.40	0.42
1:A:18:U:O2'	1:A:554:U:OP1	2.37	0.42
1:A:1026:G:H2'	1:A:1027:A:H8	1.85	0.42
12:N:12:ARG:HB3	12:N:16:HIS:HB3	2.01	0.42
1:A:244:A:H62	1:A:254:G:H21	1.66	0.42
6:F:101:ARG:NH2	6:F:139:GLU:OE2	2.52	0.42
12:N:2:ARG:HA	12:N:5:LYS:HB2	2.01	0.42
1:A:701:G:H1	1:A:731:C:H42	1.68	0.42
1:A:2722:G:H4'	12:N:4:ARG:HB2	2.02	0.42
4:D:97:SER:OG	4:D:98:VAL:N	2.53	0.42
1:A:224:U:O4	1:A:419:U:O2'	2.37	0.42
1:A:1796:U:H2'	1:A:1797:G:H8	1.84	0.42
1:A:2121:G:H1	1:A:2177:C:H42	1.66	0.42
1:A:2331:G:O3'	21:W:39:THR:OG1	2.38	0.42
1:A:2816:G:N2	1:A:2830:C:O2	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:110:THR:HG21	4:D:169:ARG:HE	1.84	0.42
9:J:24:THR:HB	9:J:27:ARG:HB2	2.01	0.42
10:K:70:ARG:HG2	10:K:76:VAL:HG22	2.01	0.42
1:A:72:U:OP2	18:T:9:LYS:NZ	2.48	0.42
1:A:1667:G:O2'	1:A:1991:U:O4	2.34	0.42
3:C:1:ALA:N	3:C:19:VAL:O	2.53	0.42
3:C:202:ARG:HE	3:C:204:LEU:HD11	1.84	0.42
15:Q:42:GLY:HA3	16:R:75:VAL:HB	2.02	0.42
15:Q:71:ASN:HD22	15:Q:109:VAL:HG21	1.84	0.42
1:A:318:C:H2'	1:A:319:G:H8	1.84	0.41
1:A:647:G:N2	1:A:2350:C:O2'	2.45	0.41
1:A:2016:U:O2	25:0:3:GLN:NE2	2.45	0.41
21:W:44:GLY:H	21:W:47:VAL:HB	1.85	0.41
1:A:2294:G:OP1	13:O:98:GLN:NE2	2.52	0.41
2:B:66:A:H61	2:B:107:G:H2'	1.84	0.41
7:G:102:ILE:HD11	7:G:116:LEU:HD11	2.02	0.41
14:P:32:VAL:HG22	14:P:37:LYS:HG2	2.02	0.41
1:A:1447:C:O2'	1:A:1544:A:N3	2.47	0.41
1:A:1494:A:H2	1:A:1579:A:H1'	1.85	0.41
1:A:1798:U:OP2	3:C:270:ARG:NH2	2.45	0.41
2:B:117:G:OP1	13:O:56:LYS:NZ	2.46	0.41
1:A:1567:G:OP1	3:C:59:GLN:NE2	2.46	0.41
1:A:1654:A:O2'	4:D:118:PHE:O	2.34	0.41
7:G:3:VAL:HG12	7:G:68:ARG:HD3	2.03	0.41
1:A:488:G:H4'	17:S:49:LYS:HE3	2.02	0.41
1:A:1446:C:O2	1:A:1545:A:O2'	2.36	0.41
18:T:48:GLN:HE22	18:T:54:GLU:HA	1.86	0.41
1:A:400:G:OP2	22:X:56:ARG:NH1	2.52	0.41
1:A:1905:C:H4'	1:A:1929:G:H8	1.86	0.41
3:C:151:GLY:O	3:C:155:ARG:NH2	2.54	0.41
8:H:28:ASN:HD21	22:X:35:HIS:CE1	2.38	0.41
20:V:9:ARG:HD3	20:V:39:ALA:HB1	2.02	0.41
1:A:121:G:H2'	1:A:122:G:H8	1.86	0.41
1:A:1420:A:O2'	1:A:2211:A:N7	2.53	0.41
1:A:16:C:H2'	1:A:17:G:H8	1.86	0.41
1:A:238:C:O2'	1:A:608:A:N3	2.47	0.41
1:A:586:A:H4'	5:E:85:PHE:HE2	1.86	0.41
1:A:1715:G:N2	1:A:1744:A:OP2	2.47	0.41
2:B:80:U:H3	2:B:96:G:H1	1.68	0.41
9:J:118:MET:HA	9:J:121:LYS:HE2	2.02	0.41
11:L:55:MET:HA	11:L:56:PRO:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:R:24:LYS:HA	16:R:94:THR:HG23	2.03	0.41
19:U:25:LYS:N	19:U:34:ILE:O	2.49	0.41
1:A:302:C:H2'	1:A:303:G:H8	1.86	0.41
1:A:1355:G:H2'	1:A:1356:G:H8	1.85	0.41
1:A:1567:G:H3'	3:C:84:PRO:HG3	2.02	0.41
4:D:48:ILE:HG23	4:D:84:LEU:HD11	2.03	0.41
14:P:21:PRO:HD3	14:P:49:ILE:HD12	2.02	0.41
22:X:13:THR:HA	22:X:27:ARG:HA	2.03	0.41
1:A:1333:G:H2'	1:A:1334:G:H8	1.86	0.40
1:A:563:A:OP2	16:R:79:ARG:NH2	2.51	0.40
1:A:1423:G:H2'	1:A:1424:G:H8	1.86	0.40
25:0:37:HIS:HB3	25:0:43:THR:HG22	2.03	0.40
1:A:136:G:H1	1:A:143:C:H42	1.69	0.40
1:A:514:A:N3	1:A:581:C:O2'	2.48	0.40
1:A:560:C:O2'	15:Q:47:ARG:NH2	2.52	0.40
1:A:1140:C:H5'	9:J:26:GLY:HA3	2.04	0.40
1:A:1578:U:H2'	1:A:1579:A:H8	1.87	0.40
4:D:33:ARG:HD3	4:D:73:VAL:HB	2.02	0.40
6:F:132:ARG:HA	6:F:150:GLY:HA2	2.02	0.40
1:A:2324:U:O2'	1:A:2337:G:OP1	2.38	0.40
6:F:105:ILE:HB	6:F:109:ARG:HH22	1.86	0.40
26:1:49:LYS:HG2	26:1:50:GLU:H	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	269/271 (99%)	252 (94%)	16 (6%)	1 (0%)	34 70
4	D	207/209 (99%)	202 (98%)	5 (2%)	0	100 100
5	E	199/201 (99%)	190 (96%)	9 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	175/177 (99%)	163 (93%)	12 (7%)	0	100	100
7	G	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
8	H	48/50 (96%)	37 (77%)	11 (23%)	0	100	100
9	J	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
10	K	120/122 (98%)	108 (90%)	12 (10%)	0	100	100
11	L	141/143 (99%)	125 (89%)	16 (11%)	0	100	100
12	N	118/120 (98%)	106 (90%)	12 (10%)	0	100	100
13	O	114/116 (98%)	107 (94%)	7 (6%)	0	100	100
14	P	112/114 (98%)	106 (95%)	6 (5%)	0	100	100
15	Q	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
16	R	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
17	S	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
18	T	91/93 (98%)	85 (93%)	6 (7%)	0	100	100
19	U	100/102 (98%)	86 (86%)	14 (14%)	0	100	100
20	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
21	W	74/76 (97%)	67 (90%)	7 (10%)	0	100	100
22	X	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
23	Y	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
24	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
25	0	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
26	1	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
27	2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
28	3	62/64 (97%)	58 (94%)	3 (5%)	1 (2%)	9	44
All	All	2898/2950 (98%)	2724 (94%)	172 (6%)	2 (0%)	54	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	12	ARG
28	3	31	ILE

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	
3	C	216/216 (100%)	216 (100%)	0	100	100
4	D	164/164 (100%)	164 (100%)	0	100	100
5	E	165/165 (100%)	165 (100%)	0	100	100
6	F	148/148 (100%)	148 (100%)	0	100	100
7	G	137/137 (100%)	137 (100%)	0	100	100
8	H	40/40 (100%)	40 (100%)	0	100	100
9	J	116/116 (100%)	116 (100%)	0	100	100
10	K	103/103 (100%)	103 (100%)	0	100	100
11	L	102/102 (100%)	102 (100%)	0	100	100
12	N	100/100 (100%)	100 (100%)	0	100	100
13	O	86/86 (100%)	86 (100%)	0	100	100
14	P	99/99 (100%)	99 (100%)	0	100	100
15	Q	89/89 (100%)	89 (100%)	0	100	100
16	R	84/84 (100%)	84 (100%)	0	100	100
17	S	93/93 (100%)	93 (100%)	0	100	100
18	T	80/80 (100%)	80 (100%)	0	100	100
19	U	83/83 (100%)	83 (100%)	0	100	100
20	V	78/78 (100%)	78 (100%)	0	100	100
21	W	56/58 (97%)	56 (100%)	0	100	100
22	X	67/67 (100%)	67 (100%)	0	100	100
23	Y	55/55 (100%)	55 (100%)	0	100	100
24	Z	48/48 (100%)	48 (100%)	0	100	100
25	0	47/47 (100%)	47 (100%)	0	100	100
26	1	45/45 (100%)	45 (100%)	0	100	100
27	2	38/38 (100%)	38 (100%)	0	100	100
28	3	51/51 (100%)	51 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2390/2392 (100%)	2390 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	36	ASN
3	C	85	ASN
3	C	152	GLN
3	C	229	HIS
3	C	238	ASN
4	D	49	GLN
4	D	134	HIS
4	D	173	GLN
5	E	62	GLN
5	E	92	HIS
6	F	51	ASN
7	G	138	GLN
8	H	28	ASN
9	J	77	HIS
10	K	3	GLN
14	P	55	HIS
15	Q	71	ASN
16	R	43	ASN
16	R	91	GLN
17	S	9	HIS
17	S	57	ASN
18	T	48	GLN
19	U	73	ASN
21	W	8	ASN
23	Y	15	ASN
24	Z	19	HIS
25	0	4	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2726/2904 (93%)	362 (13%)	10 (0%)
2	B	118/119 (99%)	11 (9%)	0
All	All	2844/3023 (94%)	373 (13%)	10 (0%)

All (373) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	12	U
1	A	34	U
1	A	35	G
1	A	45	G
1	A	46	G
1	A	63	A
1	A	71	A
1	A	74	A
1	A	75	G
1	A	84	A
1	A	103	A
1	A	118	A
1	A	120	U
1	A	125	A
1	A	138	U
1	A	139	U
1	A	140	C
1	A	141	G
1	A	142	A
1	A	181	A
1	A	196	A
1	A	199	A
1	A	216	A
1	A	221	A
1	A	222	A
1	A	230	G
1	A	248	G
1	A	255	A
1	A	265	A
1	A	266	G
1	A	271	G
1	A	272	A
1	A	276	U
1	A	278	A
1	A	302	C
1	A	311	A
1	A	322	A
1	A	329	G
1	A	330	A
1	A	331	C
1	A	353	C

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Mol	Chain	Res	Type
1	A	361	G
1	A	362	A
1	A	371	A
1	A	372	G
1	A	386	G
1	A	396	G
1	A	399	U
1	A	405	U
1	A	411	G
1	A	424	G
1	A	451	U
1	A	455	C
1	A	467	G
1	A	480	A
1	A	481	G
1	A	491	G
1	A	496	G
1	A	504	A
1	A	505	A
1	A	508	A
1	A	531	C
1	A	532	A
1	A	533	G
1	A	543	G
1	A	544	C
1	A	546	U
1	A	548	G
1	A	550	C
1	A	563	A
1	A	568	U
1	A	573	U
1	A	575	A
1	A	586	A
1	A	603	A
1	A	613	A
1	A	614	A
1	A	615	U
1	A	627	A
1	A	631	A
1	A	634	C
1	A	637	A
1	A	638	G

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Mol	Chain	Res	Type
1	A	645	C
1	A	647	G
1	A	654	A
1	A	655	A
1	A	686	U
1	A	726	G
1	A	729	G
1	A	730	A
1	A	747	U
1	A	764	A
1	A	765	C
1	A	775	G
1	A	776	G
1	A	782	A
1	A	784	G
1	A	785	G
1	A	792	A
1	A	805	G
1	A	812	C
1	A	819	A
1	A	827	U
1	A	828	U
1	A	829	A
1	A	845	A
1	A	846	U
1	A	858	G
1	A	859	G
1	A	878	A
1	A	890	C
1	A	896	A
1	A	910	A
1	A	941	A
1	A	946	C
1	A	961	C
1	A	974	G
1	A	983	A
1	A	995	C
1	A	996	A
1	A	1009	A
1	A	1012	U
1	A	1013	C
1	A	1022	G

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Mol	Chain	Res	Type
1	A	1026	G
1	A	1033	U
1	A	1046	A
1	A	1047	G
1	A	1061	U
1	A	1063	G
1	A	1065	U
1	A	1066	U
1	A	1070	A
1	A	1071	G
1	A	1072	C
1	A	1073	A
1	A	1074	G
1	A	1075	C
1	A	1088	A
1	A	1092	C
1	A	1093	G
1	A	1098	A
1	A	1104	C
1	A	1112	G
1	A	1130	U
1	A	1132	U
1	A	1133	A
1	A	1135	C
1	A	1136	G
1	A	1139	G
1	A	1142	A
1	A	1172	C
1	A	1173	U
1	A	1175	A
1	A	1176	U
1	A	1180	U
1	A	1181	U
1	A	1182	G
1	A	1206	G
1	A	1212	G
1	A	1236	G
1	A	1238	G
1	A	1250	G
1	A	1253	A
1	A	1256	G
1	A	1266	G

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Mol	Chain	Res	Type
1	A	1271	G
1	A	1272	A
1	A	1300	G
1	A	1301	A
1	A	1302	A
1	A	1306	C
1	A	1329	U
1	A	1341	G
1	A	1345	C
1	A	1365	A
1	A	1368	G
1	A	1378	A
1	A	1379	U
1	A	1383	A
1	A	1396	U
1	A	1416	G
1	A	1420	A
1	A	1428	C
1	A	1452	G
1	A	1458	U
1	A	1459	G
1	A	1482	G
1	A	1493	C
1	A	1504	A
1	A	1515	A
1	A	1523	U
1	A	1532	A
1	A	1535	A
1	A	1555	G
1	A	1566	A
1	A	1569	A
1	A	1578	U
1	A	1583	A
1	A	1585	C
1	A	1607	C
1	A	1608	A
1	A	1613	G
1	A	1647	U
1	A	1648	U
1	A	1674	G
1	A	1695	G
1	A	1715	G

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Mol	Chain	Res	Type
1	A	1730	C
1	A	1732	C
1	A	1738	G
1	A	1764	C
1	A	1773	A
1	A	1781	U
1	A	1782	U
1	A	1784	A
1	A	1786	A
1	A	1800	C
1	A	1801	A
1	A	1807	G
1	A	1808	A
1	A	1816	C
1	A	1829	A
1	A	1870	C
1	A	1873	G
1	A	1885	A
1	A	1909	C
1	A	1914	C
1	A	1925	C
1	A	1926	U
1	A	1930	G
1	A	1934	C
1	A	1936	A
1	A	1937	A
1	A	1938	A
1	A	1939	U
1	A	1940	U
1	A	1941	C
1	A	1943	U
1	A	1944	U
1	A	1945	G
1	A	1963	U
1	A	1964	G
1	A	1965	C
1	A	1966	A
1	A	1967	C
1	A	1968	G
1	A	1970	A
1	A	1972	G
1	A	1991	U

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Mol	Chain	Res	Type
1	A	1992	G
1	A	1993	U
1	A	1997	C
1	A	2022	U
1	A	2023	C
1	A	2031	A
1	A	2032	G
1	A	2043	C
1	A	2052	A
1	A	2054	A
1	A	2055	C
1	A	2056	G
1	A	2059	A
1	A	2060	A
1	A	2061	G
1	A	2064	C
1	A	2065	C
1	A	2068	U
1	A	2069	G
1	A	2072	C
1	A	2093	G
1	A	2102	G
1	A	2110	G
1	A	2111	U
1	A	2112	G
1	A	2116	G
1	A	2117	A
1	A	2118	U
1	A	2119	A
1	A	2122	U
1	A	2123	G
1	A	2128	G
1	A	2132	U
1	A	2133	G
1	A	2136	G
1	A	2147	A
1	A	2148	G
1	A	2158	A
1	A	2162	G
1	A	2164	C
1	A	2165	C
1	A	2169	A

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Mol	Chain	Res	Type
1	A	2170	A
1	A	2171	A
1	A	2172	U
1	A	2173	A
1	A	2178	C
1	A	2187	U
1	A	2198	A
1	A	2199	A
1	A	2204	G
1	A	2211	A
1	A	2212	A
1	A	2225	A
1	A	2226	C
1	A	2238	G
1	A	2239	G
1	A	2264	C
1	A	2283	C
1	A	2287	A
1	A	2297	A
1	A	2305	U
1	A	2308	G
1	A	2325	G
1	A	2327	A
1	A	2383	G
1	A	2385	C
1	A	2402	U
1	A	2406	A
1	A	2425	A
1	A	2426	A
1	A	2429	G
1	A	2430	A
1	A	2435	A
1	A	2441	U
1	A	2446	G
1	A	2448	A
1	A	2609	U
1	A	2610	C
1	A	2615	U
1	A	2629	U
1	A	2630	G
1	A	2682	A
1	A	2689	U

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Mol	Chain	Res	Type
1	A	2690	U
1	A	2714	G
1	A	2726	A
1	A	2729	G
1	A	2733	A
1	A	2744	G
1	A	2748	A
1	A	2757	A
1	A	2765	A
1	A	2766	A
1	A	2778	A
1	A	2791	G
1	A	2798	U
1	A	2800	A
1	A	2820	A
1	A	2823	A
1	A	2835	A
1	A	2836	U
1	A	2858	C
1	A	2861	U
1	A	2867	G
1	A	2872	A
1	A	2873	A
1	A	2880	C
1	A	2884	U
1	A	2886	A
2	B	13	G
2	B	15	A
2	B	24	G
2	B	35	C
2	B	36	C
2	B	41	G
2	B	56	G
2	B	66	A
2	B	90	C
2	B	99	A
2	B	109	A

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	271	G

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Mol	Chain	Res	Type
1	A	404	A
1	A	995	C
1	A	1344	U
1	A	1378	A
1	A	1938	A
1	A	2060	A
1	A	2127	G
1	A	2425	A
1	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.

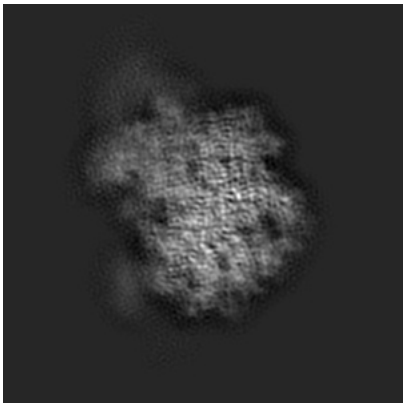
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4379. These allow visual inspection of the internal detail of the map and identification of artifacts.

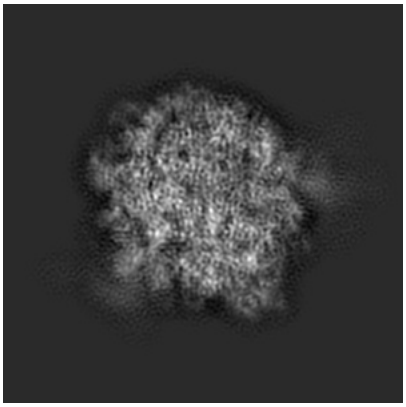
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

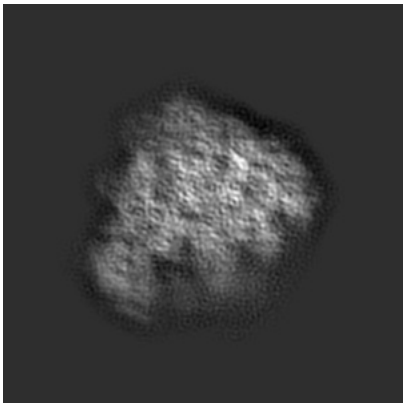
6.1.1 Primary map



X



Y

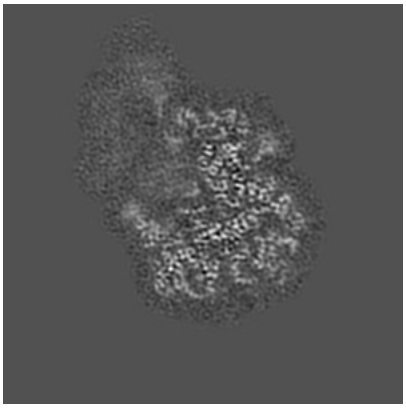


Z

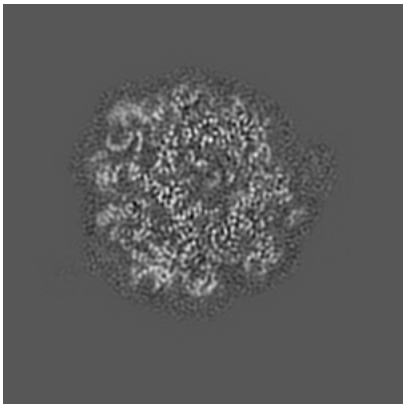
The images above show the map projected in three orthogonal directions.

6.2 Central slices

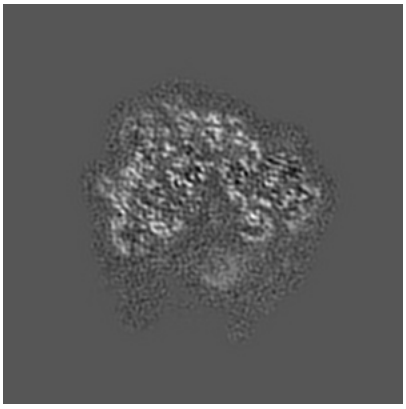
6.2.1 Primary map



X Index: 135



Y Index: 135

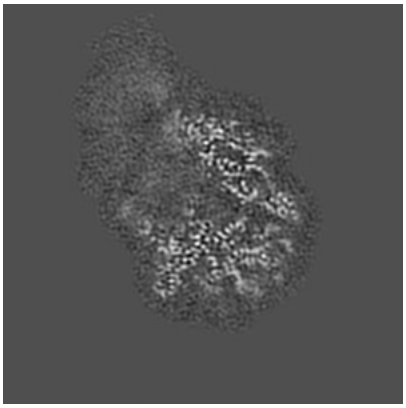


Z Index: 135

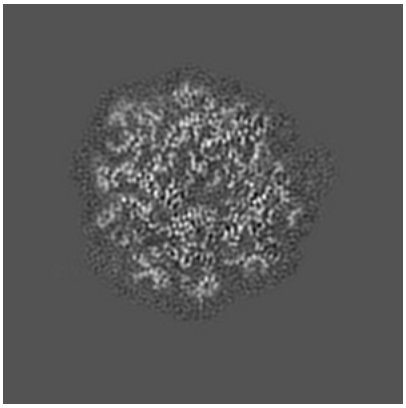
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

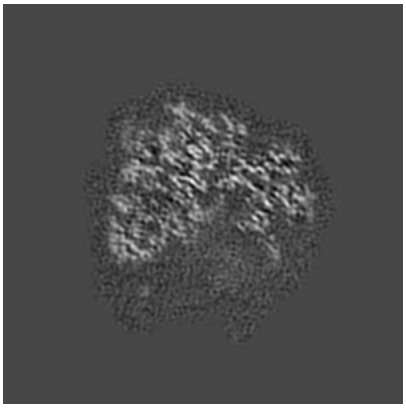
6.3.1 Primary map



X Index: 140



Y Index: 137



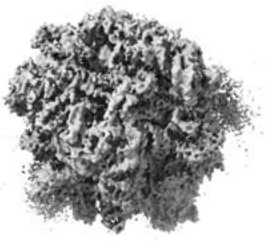
Z Index: 140

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 4.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

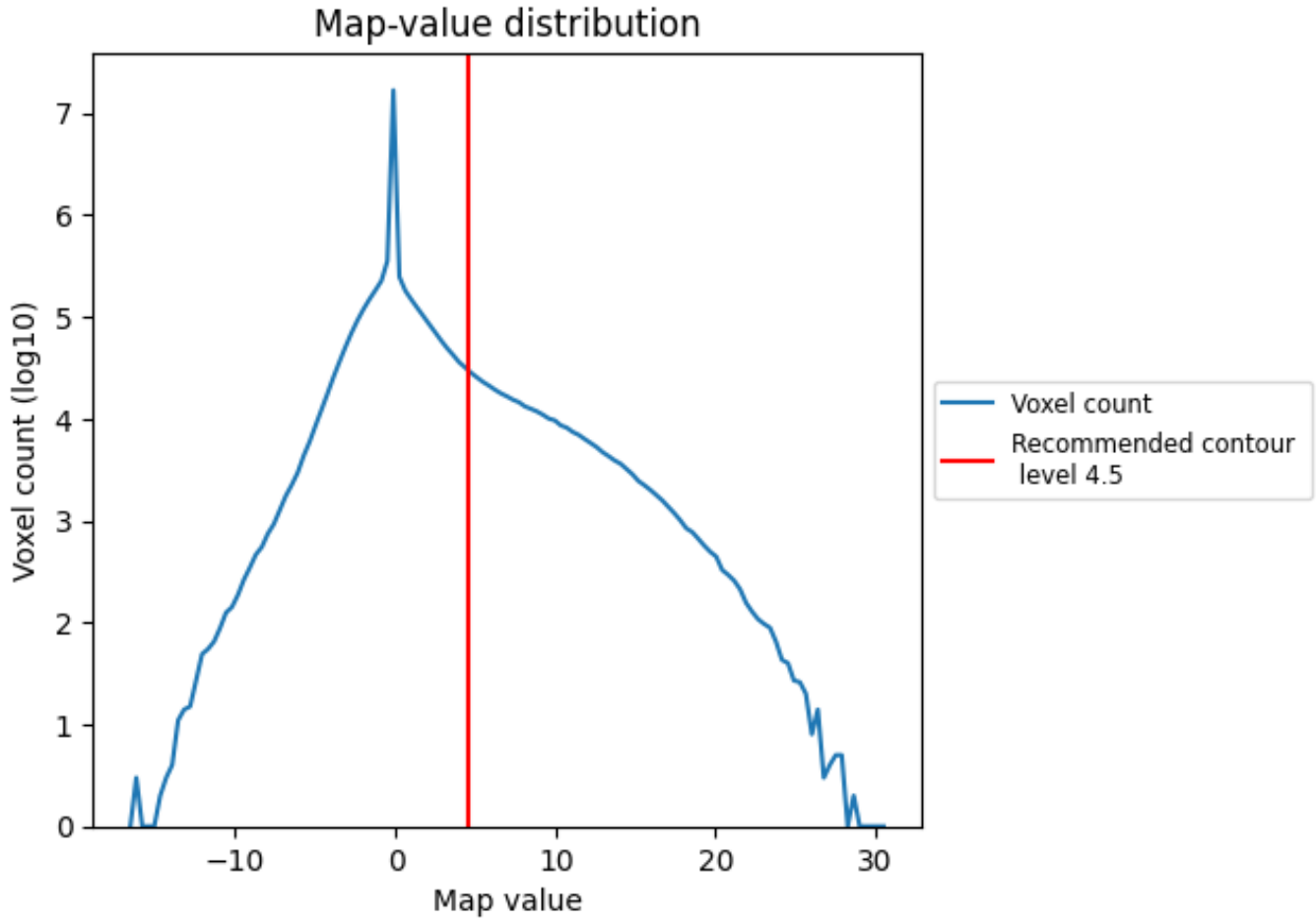
6.5 Mask visualisation (i)

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

7 Map analysis

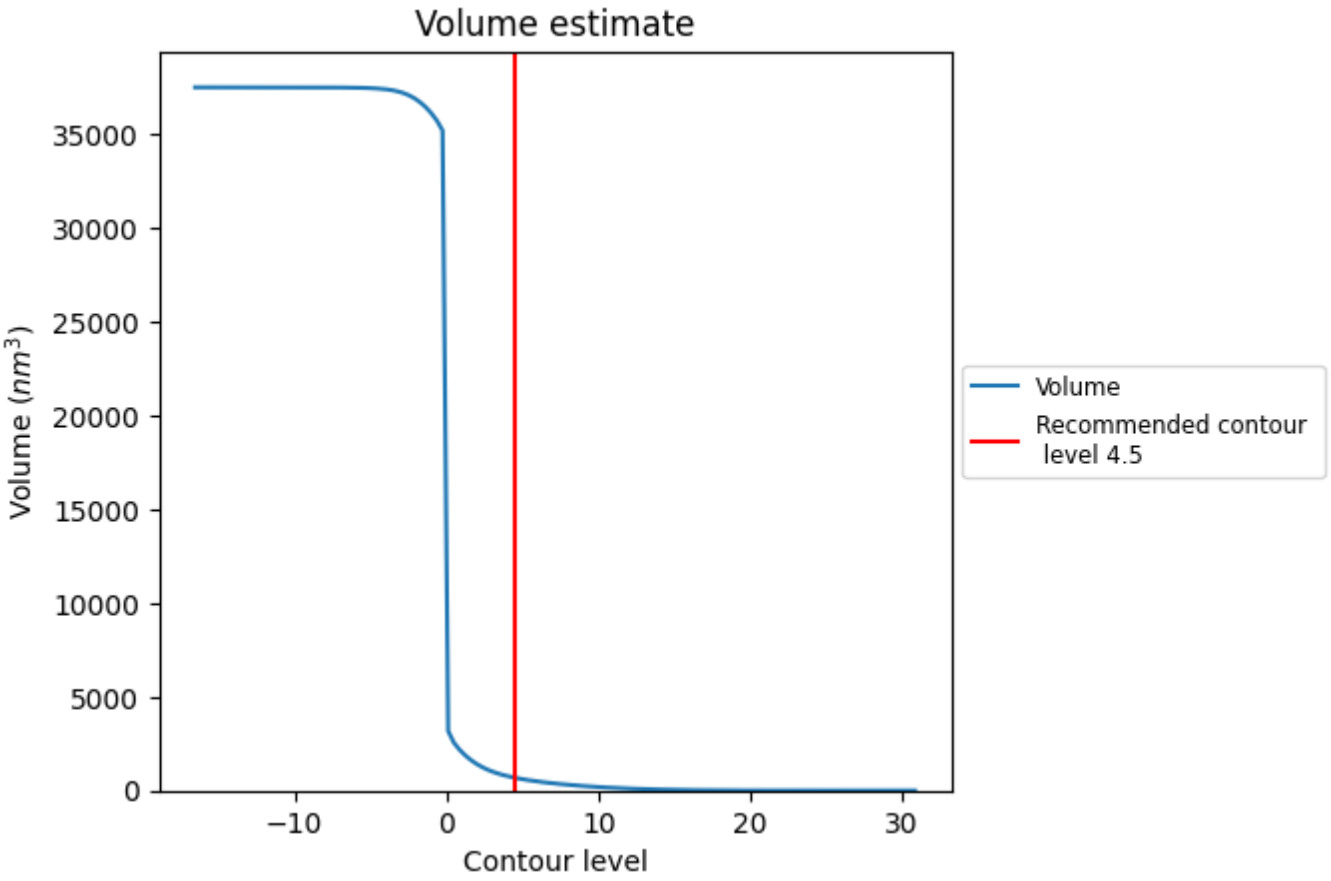
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

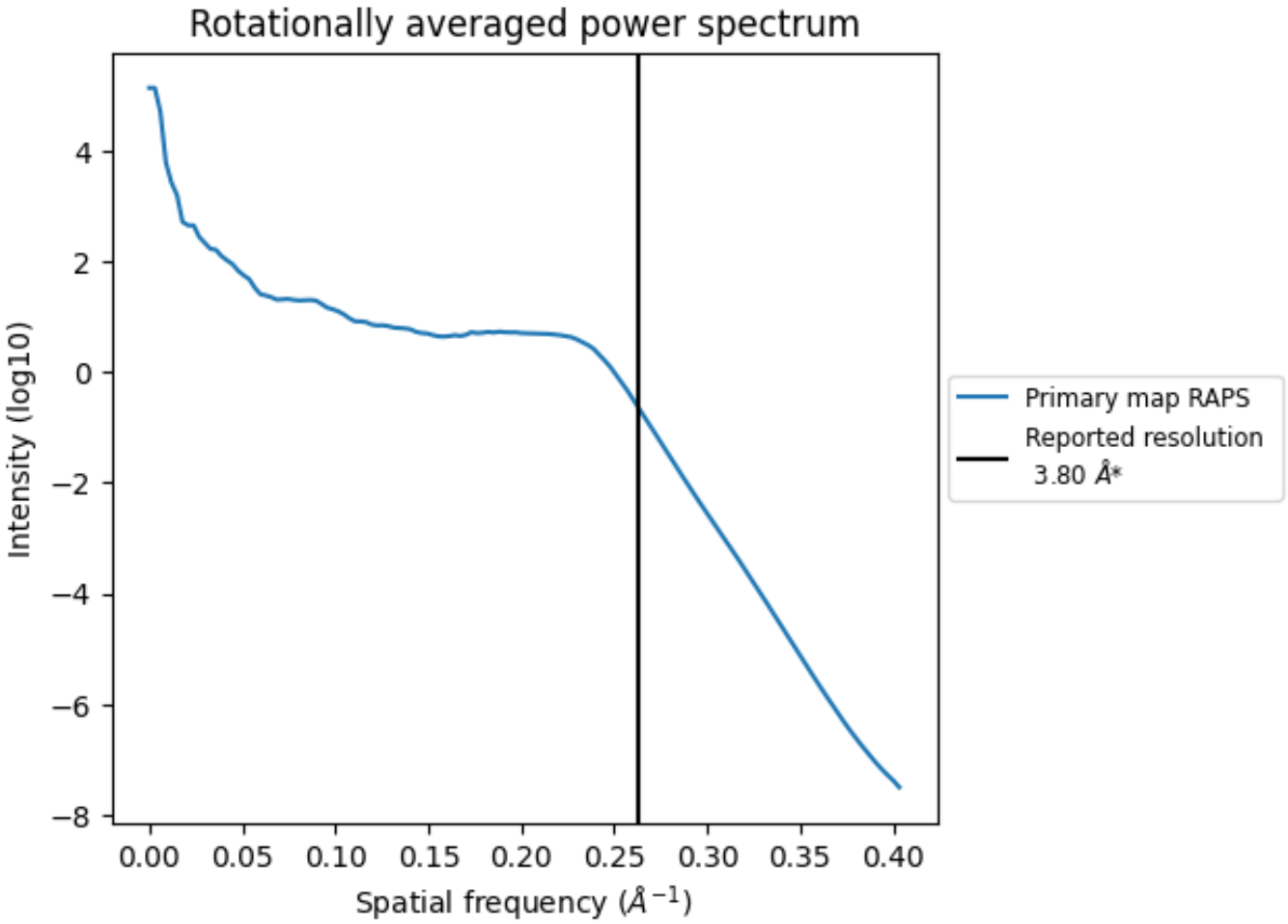
7.2 Volume estimate



The volume at the recommended contour level is 686 nm^3; this corresponds to an approximate mass of 620 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 (i)



*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

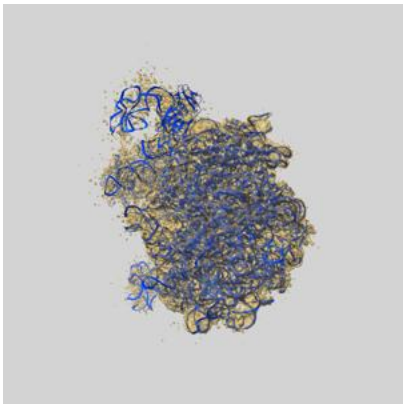
8 Fourier-Shell correlation

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

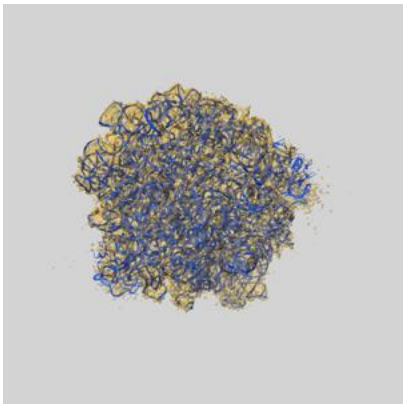
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4379 and PDB model 6GC0. Per-residue inclusion information can be found in section 3 on page 9.

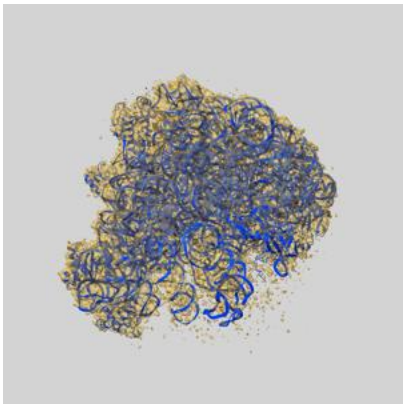
9.1 Map-model overlay



X



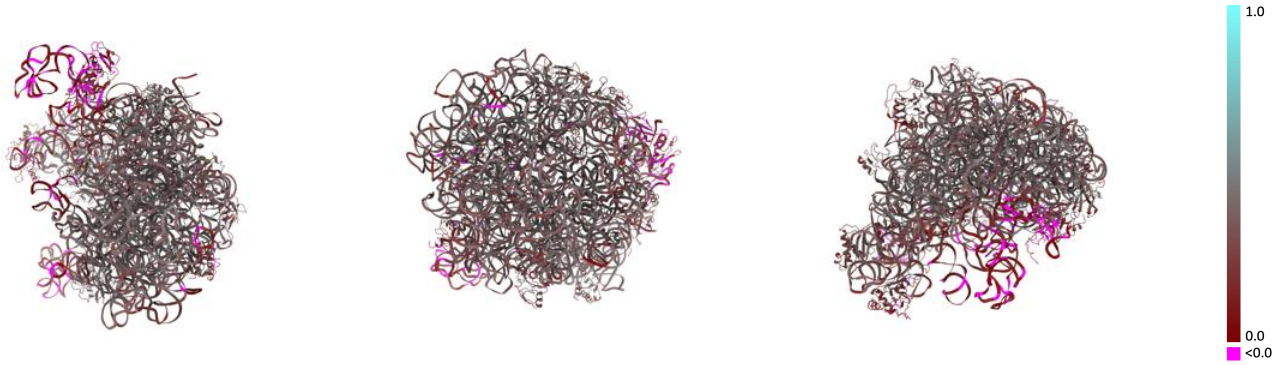
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

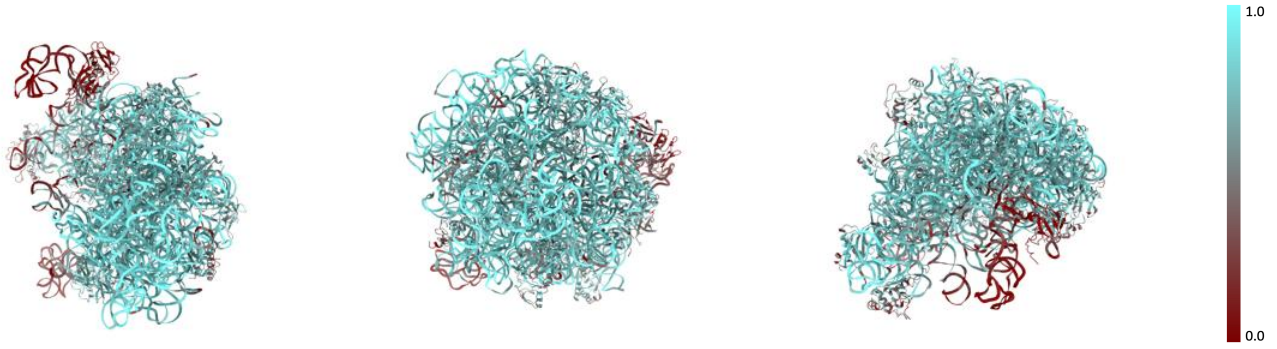
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

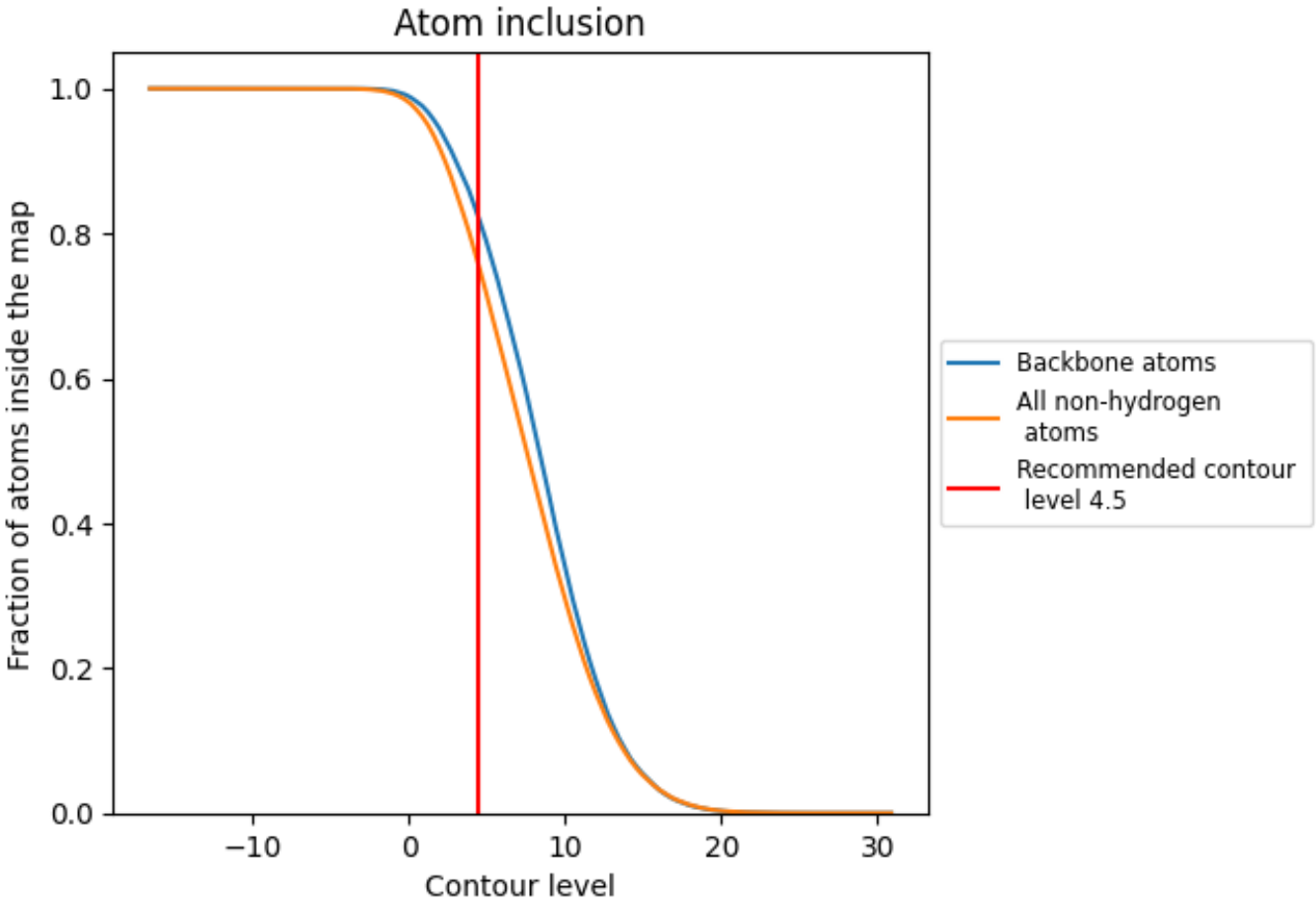
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (4.5).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 75% 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 (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7541	0.3410
0	0.7009	0.3630
1	0.5199	0.3160
2	0.7493	0.3970
3	0.7047	0.4050
A	0.8045	0.3500
B	0.8340	0.3350
C	0.7134	0.3830
D	0.6359	0.3390
E	0.6013	0.3110
F	0.4854	0.2110
G	0.0702	0.0510
H	0.3219	0.2330
J	0.7100	0.3740
K	0.6433	0.3190
L	0.6594	0.3500
N	0.7183	0.3810
O	0.6698	0.2920
P	0.6610	0.3300
Q	0.7489	0.3850
R	0.6863	0.3530
S	0.6998	0.3820
T	0.6680	0.3350
U	0.6380	0.3110
V	0.5108	0.2610
W	0.7030	0.3760
X	0.7188	0.3760
Y	0.4547	0.2560
Z	0.6911	0.4010