

wwPDB EM Validation Summary Report (i)

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PDB ID	:	5H1S
EMDB ID	:	EMD-9572
Title	:	Structure of the large subunit of the chloro-ribosome
Authors	:	Ahmed, T.; Yin, Z.; Bhushan, S.
Deposited on	:	2016-10-11
Resolution	:	3.50 Å(reported)

This is a wwPDB EM Validation Summary 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 (i) 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 (1)) were used in the production of this report:

:	0.0.1. dev 43
:	4.02b-467
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	1.9.9
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	2.31.2
	: : : : :

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM\ structures}\ (\#{ m Entries})$
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 $\geq=3, 2, 1$ 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	Q	uality of chain		
1	А	2810	29%	43%		27%
2	С	106	6% 9% 46%		37%	. .
3	В	121	1 2% 43%		40%	
4	L	191	36%	39%		23%
5	М	121	17%		46%	
6	Ν	192	9%	51%		9% • 8%
7	О	135	16%		54%	••

Continued on next page...



Chain Length Quality of chain Mol 8 Р 11657% 43% 15% •• 9 Q 12341% 55% 12% 10 R 15632% 41% 24% ... 6% \mathbf{S} 11 12744% 45% 9% • 14% Т 1220128% 38% 5%• 27% 13% 13U 19934% 28% 37% • 12% V 1221433% 40% 25% • 21% W 1514536% 46% 14% •• 10% Х 1371628% 27% 36% 9% 5% Υ 177747% 43% 6% 15% Ζ 1810936% 44% 17% • 10% Е 1927141% 47% 9% • 5% 20 \mathbf{b} 5682% 18% 15% 21 \mathbf{c} 6575% 22% . 13% 22 \mathbf{d} 60 7% 5% 88% 2373е • 5% 90% 5% f 24• 3797% 7% F 2522144% 49% • • 11% G 2624332% 50% 5% 14% 56% Η 2202735% 43% 20% • 21% Ι 2818252% • 5% 42% 26% 29J 15518% 15% 66% 8% 14230 30% 70% g • 39% 9431 \mathbf{a} 38% 60% 32h 11635% 60%





2 Entry composition (i)

There are 32 unique types of molecules in this entry. The entry contains 90825 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues			AltConf	Trace			
1	А	2799	Total 60117	C 26819	N 11134	O 19365	Р 2799	0	0

• Molecule 2 is a RNA chain called Spinach chloroplast 4.5S rRNA.

Mol	Chain	Residues		Α	AltConf	Trace			
2	С	102	Total 2187	C 977	N 403	O 705	Р 102	0	0

• Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues		A	AltConf	Trace			
3	В	117	Total 2500	C 1116	N 452	0 815	Р 117	0	0

• Molecule 4 is a protein called 50S ribosomal protein L13, chloroplastic.

Mol	Chain	Residues		At	oms	AltConf	Trace		
4	L	147	Total 1184	C 754	N 225	O 202	${ m S} { m 3}$	0	0

• Molecule 5 is a protein called 50S ribosomal protein L14, chloroplastic.

Mol	Chain	Residues		At	oms	AltConf	Trace		
5	М	121	Total 942	C 588	N 179	0 170	${S \atop 5}$	0	0

• Molecule 6 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues		At	oms		AltConf	Trace	
6	Ν	177	Total 1342	C 836	N 264	O 236	S 6	0	0



• Molecule 7 is a protein called 50S ribosomal protein L16, chloroplastic.

Mol	Chain	Residues		At	\mathbf{oms}	AltConf	Trace		
7	Ο	134	Total 1067	C 672	N 217	0 173	${ m S}{ m 5}$	0	0

• Molecule 8 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues		At	oms	AltConf	Trace		
8	Р	116	Total 944	C 592	N 193	0 155	$\frac{S}{4}$	0	0

• Molecule 9 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues		At	oms		AltConf	Trace	
9	Q	120	Total 947	C 589	N 183	0 170	${f S}{5}$	0	0

• Molecule 10 is a protein called 50S ribosomal protein L19, chloroplastic.

Mol	Chain	Residues		At	\mathbf{oms}	AltConf	Trace		
10	R	118	Total 953	C 610	N 186	0 156	S 1	0	0

• Molecule 11 is a protein called 50S ribosomal protein L20, chloroplastic.

Mol	Chain	Residues		At	oms		AltConf	Trace	
11	S	115	Total 996	C 633	N 208	0 153	$\frac{S}{2}$	0	0

• Molecule 12 is a protein called 50S ribosomal protein L21, chloroplastic.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
12	т	147	Total	С	Ν	Ο	0	0
14	T	141	1171	759	202	210	0	0

• Molecule 13 is a protein called 50S ribosomal protein L22, chloroplastic.

Mol	Chain	Residues		At	oms	AltConf	Trace		
13	U	144	Total 1149	C 731	N 210	O 200	S 8	0	0

• Molecule 14 is a protein called 50S ribosomal protein L23, chloroplastic.



Mol	Chain	Residues		At	oms			AltConf	Trace
14	V	92	Total 740	C 477	N 129	0 132	${ m S} { m 2}$	0	0

• Molecule 15 is a protein called 50S ribosomal protein L24, chloroplastic.

Mol	Chain	Residues		At	oms	AltConf	Trace		
15	W	124	Total 993	C 624	N 187	O 180	${S \over 2}$	0	0

• Molecule 16 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
16	Х	100	Total 810	C 511	N 159	O 140	0	0

• Molecule 17 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
17	Y	74	Total	C	N	0	S	0	0
			605	385	121	98	1		

• Molecule 18 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues		At	oms	AltConf	Trace		
18	Ζ	90	Total 754	C 470	N 150	0 131	${ m S} { m 3}$	0	0

• Molecule 19 is a protein called 50S ribosomal protein L2, chloroplastic.

Mol	Chain	Residues		At	AltConf	Trace			
19	Е	247	Total 1904	C 1181	N 390	O 327	S 6	0	0

• Molecule 20 is a protein called 50S ribosomal protein L32, chloroplastic.

Mol	Chain	Residues		Atom	ıs	AltConf	Trace	
20	b	46	Total 378	C 250	N 70	O 58	0	0

• Molecule 21 is a protein called 50S ribosomal protein L33, chloroplastic.



Mol	Chain	Residues		Atc	\mathbf{ms}			AltConf	Trace
21	с	51	Total 415	C 258	N 83	O 70	$\frac{S}{4}$	0	0

• Molecule 22 is a protein called 50S ribosomal protein L34, chloroplastic.

Mol	Chain	Residues		Ate	oms	AltConf	Trace		
22	d	57	Total 445	C 268	N 103	0 71	${ m S} { m 3}$	0	0

• Molecule 23 is a protein called 50S ribosomal protein L35, chloroplastic.

Mol	Chain	Residues		Ate	oms	AltConf	Trace		
23	е	69	Total 563	C 353	N 119	O 90	${f S}$ 1	0	0

• Molecule 24 is a protein called 50S ribosomal protein L36, chloroplastic.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
24	f	37	Total 304	C 186	N 70	0 44	$\frac{S}{4}$	0	0

• Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues		At	oms			AltConf	Trace
25	F	212	Total 1620	C 1025	N 295	0 289	S 11	0	0

• Molecule 26 is a protein called 50S ribosomal protein L4, chloroplastic.

Mol	Chain	Residues		At	oms			AltConf	Trace
26	G	210	Total 1655	C 1052	N 308	O 292	${ m S} { m 3}$	0	0

• Molecule 27 is a protein called 50S ribosomal protein L5, chloroplastic.

Mol	Chain	Residues		At	oms			AltConf	Trace
27	Н	175	Total 1351	C 862	N 233	0 248	S 8	0	0

• Molecule 28 is a protein called 50S ribosomal protein L6.



Mol	Chain	Residues		At	oms			AltConf	Trace
28	Ι	173	Total 1353	$\begin{array}{c} \mathrm{C} \\ 855 \end{array}$	N 249	0 245	$\frac{S}{4}$	0	0

• Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
29	J	53	Total 423	C 280	N 74	O 68	S 1	0	0

• Molecule 30 is a protein called 50S ribosomal protein 5 alpha, chloroplastic.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
30	g	43	Total 345	C 218	N 65	O 59	${f S}\ 3$	0	0

• Molecule 31 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues		Ato	\mathbf{ms}			AltConf	Trace
31	a	38	Total 300	C 187	N 49	O 62	$\frac{S}{2}$	0	0

• Molecule 32 is a protein called 50S ribosomal protein 6, chloroplastic.

Mol	Chain	Residues		Ato	\mathbf{ms}			AltConf	Trace
32	h	46	Total 368	C 237	N 71	O 59	S 1	0	0



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 rRNA





C1554 G1555 A1556	G1557 U1558 A1559	A1562 G1566	C1567 U1568	C1570 G1571 G1572	C1573 G1574 C1575	U1576 G1577 A1578	A1579 G1580 U1581	A1582 A1583 C1584	C1585 G1586 A1587	U1588 G1589 C1590	C1591 A1592 M1000	01593 A1594 C1595	01596 C1597 C1509	C1598 C1599 A1600	<mark>G1601</mark> G1602 A1603	A1604 A1605 A1606	G1607 C1608	01609 C1610 G1611	A1612 A1613	C1614 G1615 A1616						
C1617 C1618 U1619	U1620 C1621 A1622	A1523 C1624 A1625	A1627 A1628	G1630 G1631 U1632	A1633 C1634 C1635	01636 G1637	G1643 A1644 A1645 A1646	C1647 C1648 C1648	G1650 C1651	A1652 C1653 <mark>A1654</mark>	G1655 A1662	G1663 G1664	01665 A1666 G1667	A1668 G1669 A1670	A1671 U1672 A1673	C1674 C1674 C1675		G1683 C1684	G1687 A1688	C1689 A1690						
A1691 C1692 U1693	C1694 U1697 C1698	U1699 A1700 A1701	61702 61703 A1704 A1705	C1706 61709	61710 C1711 A1712	A1/15 A1714 A1715 11716	61710 61717 61718	G1723	G1731 G1732 G1732	61 733 A1 734 G1 735	A1736 A1737 G1738	G1739 G1740	G1743 C1744	C1745 C1746 C1747	C1748 U1749	C1750 A1751	C1752 A1753	A1754 A1755	G1757 G1757 G1758	<mark>G1759</mark> G1760						
G1763 G1766	<mark>U1767</mark> G1768 A1769 C1770	G1774 C1775 C1775	C1776 C1777 G1778	C1781 G1782 A1783	G1786	01/09 A1793	A1795 A1795 A1796 A1797	C1798 A1799 C1800	A1801 61802	G1803 U1804 C1805	U1806 C1807 C1808	G1809 C1810 A1811	A1611 A1812 A1813	G1814 U1815 C1816	<mark>G1817</mark> U1818 A1819	A1820 G1821 A1822	C1823 C1823 C1824	A1825 U1826 C1827	U1828 A1829	U1830						
61831 61832 61833	61834 61835 C1836 U1837	G1838 A1839 C1840	61041 C1842 C1847	C1848 A1849 G1850	01851 61852 C1853	A1857 A1858 A1858	G1859 G1860 U1861	G1866 A1867	A1868 G1869 U1870	U1871 <mark>G1872</mark> G1873	U1874 G1875 A1876	C1877 C1878	01879 G1880 A1881	U1882 G1883	A1884 C1885 A1886	G1887 G1888 G1888	61890 61890 A1891	61892	61895 61896 01897	G1898						
61902 61910	A1914 A1915 C1916	G1917 G1920	C1922	01925 A1926 A1927	C1928 U1929 A1930	U1931 A1932	A1933 G1936 H1 027	C1938 C1938 C1939	U1940 A1941 A1942	G1943 G1944 U1945	G1949 A1950	A1951 A1952	U1953 U1954 C1955	C1956 U1957 U1958	G1959 U1960	U1965 A1966	A1967 G1968 U1969	U1970 C1971		G1978 C1979	OSETH					
C1981 G1982 <mark>A1983</mark>	A1984 A1985 G1986 G1987	C1988 G1989	61994 61994 61999	A2003 C2004	U2005 G2006 U2007	C2010 C2010 C2011	G2012 A2013 G2014	A2015 G2016 A2017	G2019	G2024 U2025	G2026 A2027	A2033 C2034 A2035	42035 U2036 G2037	U2038 C2039 U2040	G2041	A2045 G2046 A2047	02048 02049 02049	C2050 G2051	C2054 U2055	A2056						
C2057 C2058 U2059	G2060 C2061 A2062	U2065 G2066		A2074 G2075 A2076	C2077 C2078 C2079	G2083 A2084	U2089 U2089 U2090	A2091 G2094		G2103 A2104 U2105	U2106 G2107 G2108	C2109 U2110	U2111 U2112	G2113 G2114	G2115 C2116 10117	U2116 U2118 U2119A	U2120 C2121	C2122 U2123	G2124 C2125	G2126 C2127	A2128 G2129	C2130				
U2131 U2132	A2133 G2134 G2135	U2136 G2137 G2138	A2139 A2140 G2141	G2142 C2143	G2144 A2145 A2146	G2147 A2148	A2149 G2150 G2151	c2152 c2153	C2154 C2155	C2156 U2157	U2158 C2159	G2161	G2162 G2163	G2164 G2165	62167 C2168	c2169 C2170	G2171 +	G2173 C2174	C2175 A2176	U2177	A2179 G2180	U2181 G2182	A2183 G2184	A2185 U2186	A2107 C2188 C7189	20120
C2191 U2192	C2193 U2194 G2195	G2196 A2197 A2198	G2199 A2200 G2201	C2202 U2203 A2204	G2205 A2206	12208 12208 12209	02210 U2211 A2212 A2213	C2214 C2215 112216	02210 U2217 G2218	U2219 G2220 U2221	C2222 A2223 G2224	G2225 A2226	C2227 C2228 IIC228	A2230 C2231 C2231	G2232 G2233 G2234	C2235 C2236 A2237	A2238 G2239	62241 62241 A2242	C2243 A2244	C2247 U2248	C2249					
G2255 A2256	U2260 U2261 U2262 C2263	U2264 A2265 U2266	62.268 62.268 U2273	<mark>A2274</mark> G2275 G2276	C2277 C2278 U2279	A2283	A2 20 4 A2 285 A2 286 G2 287	G2288 U2289 A2290	A2291 C2292	62293 62294 A2295	G2296 G2297	U2300 G2301 C2302	A2302 A2303 A2304	A2305 G2306 G2307	U2308 U2309 U2310	C2311 C2312 U2312	C2314 C2315 G2315	G2316 G2317 C2318	C2319 C2319 G2320	G2321						
A2322 C2323	G2324 G2325 A2326	G2327 A2328 U2329	02330 G2331 G2332 C2333	C2334 C2335	C2337 G2338 A2330	G2340 U2341 G2342	C2343 A2344 A2345	A2346 G2347	A2350 G2351	A2352 A2353 G2354	G2355 G2358	C2359 U2360	<mark>02361</mark> G2362 A2363	C2364 C2367	C2372	C2374 C2374 A2375	02376 C2377 C2378	C2381	G2389	A2390 A2393	A2394					
A2395 G2396 U2397	<mark>C2398</mark> G2399 G2400 C2401	C2402 U2403	62400 62408 A2409	U2410 C2411	A2414 C2415 G2416	62419 02418 62419	C2420 C2421 G2422	62425 02425 02425	G2426 G2427 A2428	A2429 G2430 G2431	G2432 C2433 C2434	C2437	<mark>G 2438</mark> C2439 U2440	C2441 A2442 A2443	C2444 G2445	42447	A2451 A2452	C2457 U2458	G2462 G2463	G2464						













 \bullet Molecule 16: 50S ribosomal protein L27







• Molecule 26: 50S ribosomal protein L4, chloroplastic





• Molecule 29: 50S ribosomal protein L9

	26%						
Chain J:	18%	15% •		66%			
****		*****	** *****	• • •	• • • •	*****	•••
GLN K43 K44 K46 V45 K46 K47 K47 I48	R49 K50 I51 I52 L53 K54	E55 D56 157 P58 D59 L60 C61	K62 K63 G64 G65 L65 L67 D68 D68 V69	A71 672 F73 L74 R75 N76 F77 F77 L78 L78 L78 L78 L81	682 682 884 884 885 V86 V86	Т88 Р89 L90 L92 V92	E94 E94 M95 NET ASP GLU GLU ARG
ILE GLU GLU GLU LYS LYS ARG VAL LYS	GLU GLU GLU GLN GLN LLEU ALA ARG	MET PHE GLU THR VAL CLY ALA ALA PHE	LYS VAL LYS ARG LYS GLY CLYS CLY CLYS CLN	ILE PHE GLY SER VAL THR ALA ALA ASP LLU LLU VAL ASP	TLE TLE LYS ALA GLN CGLN CGLN	ARG ASP VAL ASP LYS	
LYS VAL VAL PHE LEU PRO ASP ILE ARG	GLU THR GLY GLU TYR ILE ALA GLU	LEU LYS LEU HIS PRO ASP VAL THR	ALA GLN VAL ARG VAL THR VAL VAL PHE ALA ASN				
• Molecule 3	30: 50S rib	osomal prot	tein 5 alpha, ch	loroplastic			
Chain g:	% 30%	·		70%			
MET ALA LEU LEU SER PRO LEU LEU SER	LEU SER SER VAL PRO TLE THR	SER ILE ALA VAL SER SER SER SER	PHE PRO TLE LYS LYS LEU GLN GLN ASN SER VAL SER ALA	LEU LEU PRO SER PHE GLY GLN ARC LEU VAL ALA HTS	GLY PRO VAL ILE ALA GLN LYS	ARG GLY THR VAL VAL	
		• •	• •• ••••	• ••			
ALA MET VAL SER ALA ALA ALA GLU GLU	THR ALA GLY GLU GLU ASP ASP GLN	K79 K79 N89 L90 E93	M106 1112 1112 1113 1114 1115 1117 7117 7117	L119 L119 C120 L12 A121 L12 G12 A121 L12 L12 L12 ARG A17 C17 C17 C17 C17 C17 C17 C17 C17 C17 C	ALA TRP PRO PRO SER LYS MET	LYS LYS LEU LYS ASN VAL	
• Molecule 3	31: 50S rib	osomal prot	tein L31				
Chain a:	399 389	%		60%			
	*****	******	******	•••••	•		
ARG K38 S39 D40 141 H42 H42 P43	E44 F45 R46 E47 D48 A49	K50 V51 Y52 C53 N54 G55 G55	L57 L57 M59 M59 T60 T61 G62 G63 T64	q65 K66 D67 Y68 Y68 T69 V70 E71 V72 V72	S74 G75 ASN HIS PRO PHE TYR	LEU GLY ASN ARG SER ALA LEU LEU	LEU ASP ALA ASP ASP GLN VAL GLU CLU LYS
PHE ARG LYS LYS LYR GLY GLU LEU THR	GLN ILE MET GLU ILE PRO VAL LEU	LYS GLY GLV GLU ILE LEU PRO PRO	LYS LYS LYS SER LYS ALA LYS LYS LYS LYS				
• Molecule 3	32: 50S rib	osomal prot	tein 6, chloropla	astic			
Chain h:	35%			60%			
						•	
MET SER VAL SER ALA TLE PHE GLY ALA	ARG VAL VAL THR THR TLE PRO SER VAL	LEU ARG THR SER SER VAL ASP GLY	ARG THR VAL LYS LYS LLYS GLN PRO SER SER GLY GLY	SER CYS GLY GLY GLY GLY VAL THR THR THR THR THR THR S48	849 R50 W70 K73	V78 Y79 L85	
•							
V92 S93 SER ALA VAL ASP GLU ASP	SER SER SER THR THR SER	SER SER ALA GLU TLE ALA GLN SER ALA					



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	174949	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{\AA}^2)$	26	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	109375	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.928	Depositor
Minimum map value	-0.585	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.132	Depositor
Map size (Å)	399.36, 399.36, 399.36	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.28, 1.28, 1.28	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).

Mal	Chain	Bo	ond lengths	Bond angles			
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5		
1	А	0.80	18/67340~(0.0%)	0.94	109/105056~(0.1%)		
2	С	3.05	9/2449~(0.4%)	1.30	26/3817~(0.7%)		
3	В	0.78	0/2796	0.87	2/4357~(0.0%)		
4	L	0.67	0/1212	0.68	1/1634~(0.1%)		
5	М	0.60	0/951	0.69	1/1282~(0.1%)		
6	Ν	0.40	0/1361	0.77	3/1806~(0.2%)		
7	0	0.63	1/1089~(0.1%)	0.71	1/1461~(0.1%)		
8	Р	0.63	0/959	0.76	0/1280		
9	Q	0.52	0/963	0.67	0/1293		
10	R	0.61	0/967	0.79	2/1300~(0.2%)		
11	S	0.77	0/1013	0.82	1/1351~(0.1%)		
12	Т	0.73	0/1199	0.88	3/1633~(0.2%)		
13	U	0.60	1/1168~(0.1%)	0.69	0/1566		
14	V	0.53	0/749	0.65	0/1006		
15	W	0.49	0/1006	0.67	2/1343~(0.1%)		
16	Х	0.66	0/825	0.80	2/1099~(0.2%)		
17	Y	0.65	0/615	0.78	2/819~(0.2%)		
18	Ζ	0.52	0/762	0.71	0/1012		
19	Е	0.60	0/1938	0.78	1/2603~(0.0%)		
20	b	0.72	0/387	0.65	0/513		
21	с	0.55	0/422	0.85	1/564~(0.2%)		
22	d	0.45	0/447	0.63	0/588		
23	е	0.72	0/569	0.82	1/752~(0.1%)		
24	f	0.57	0/306	0.78	0/403		
25	F	0.66	0/1646	0.74	1/2201~(0.0%)		
26	G	0.65	2/1687~(0.1%)	0.78	1/2271~(0.0%)		
27	Н	0.37	0/1372	0.60	0/1848		
28	Ι	0.49	0/1374	0.63	1/1849~(0.1%)		
29	J	0.33	0/427	0.65	0/568		
30	g	0.44	0/345	0.85	1/455~(0.2%)		
31	a	0.29	0/306	0.60	0/413		
32	h	0.70	1/382~(0.3%)	0.81	2/520~(0.4%)		
All	All	0.88	32/99032~(0.0%)	0.90	$16\overline{4/148663}~(0.1\%)$		



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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	Q	0	1
10	R	0	1
11	S	0	3
13	U	0	1
19	Е	0	3
24	f	0	1
25	F	0	1
26	G	0	2
27	Н	0	1
32	h	0	2
All	All	0	16

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	С	95	А	N3-C4	76.76	1.80	1.34
2	С	95	А	C6-N1	71.09	1.85	1.35
2	С	95	А	C5-C4	50.90	1.74	1.38
2	С	95	А	C2-N3	47.29	1.76	1.33
2	С	95	А	N1-C2	47.04	1.76	1.34

The worst 5 of 164 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	95	A	N1-C2-N3	-28.24	115.18	129.30
2	С	95	A	C2-N3-C4	24.30	122.75	110.60
2	С	95	A	N7-C8-N9	14.45	121.03	113.80
6	N	196	LEU	C-N-CD	-14.44	88.83	120.60
2	С	95	А	C4-C5-N7	-13.30	104.05	110.70

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	Q	70	ARG	Peptide
10	R	190	VAL	Peptide
11	S	24	PHE	Peptide
11	S	82	ILE	Peptide



Continued from previous page...

Mol	Chain	Res	Type	Group
11	S	96	ILE	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	А	60117	0	30254	3962	0
2	С	2187	0	1099	306	0
3	В	2500	0	1263	331	0
4	L	1184	0	1221	135	0
5	М	942	0	996	51	0
6	Ν	1342	0	1413	392	0
7	0	1067	0	1120	103	0
8	Р	944	0	1004	68	0
9	Q	947	0	966	87	0
10	R	953	0	1044	80	0
11	S	996	0	1060	122	0
12	Т	1171	0	1216	216	0
13	U	1149	0	1220	98	0
14	V	740	0	795	103	0
15	W	993	0	1054	127	0
16	Х	810	0	847	185	0
17	Y	605	0	652	51	0
18	Ζ	754	0	804	99	0
19	Ε	1904	0	1982	219	0
20	b	378	0	413	0	0
21	с	415	0	434	0	0
22	d	445	0	501	0	0
23	е	563	0	621	0	0
24	f	304	0	342	0	0
25	F	1620	0	1699	174	0
26	G	1655	0	1723	238	0
27	Н	1351	0	1407	136	0
28	Ι	1353	0	1416	90	0
29	J	423	0	488	39	0
30	g	345	0	395	0	0
31	a	300	0	279	0	0
32	h	368	0	386	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	90825	0	60114	6418	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 46.

The worst 5 of 6418 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2351:G:C4	9:Q:64:VAL:HG21	1.27	1.61
2:C:95:A:C5	2:C:95:A:C6	1.79	1.59
16:X:128:TYR:CB	16:X:134:LYS:CD	1.78	1.58
11:S:91:LEU:CD1	12:T:175:PRO:HB3	1.30	1.55
1:A:274:G:C6	1:A:433:C:C6	1.94	1.54

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	Perce	entiles
4	L	145/191~(76%)	120 (83%)	21 (14%)	4 (3%)	5	32
5	М	119/121~(98%)	97~(82%)	22 (18%)	0	100	100
6	Ν	175/192~(91%)	156 (89%)	6 (3%)	13 (7%)	1	11
7	Ο	132/135~(98%)	107 (81%)	23~(17%)	2 (2%)	10	45
8	Р	114/116~(98%)	96 (84%)	18 (16%)	0	100	100
9	Q	118/123~(96%)	99 (84%)	19 (16%)	0	100	100
10	R	116/156~(74%)	89 (77%)	26 (22%)	1 (1%)	17	56
11	S	113/127~(89%)	91 (80%)	22 (20%)	0	100	100
12	Т	145/201~(72%)	108 (74%)	28 (19%)	9 (6%)	1	15



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
13	U	142/199~(71%)	117 (82%)	24 (17%)	1 (1%)	22	61
14	V	90/122~(74%)	79 (88%)	9 (10%)	2 (2%)	6	37
15	W	122/145~(84%)	95 (78%)	25 (20%)	2 (2%)	9	43
16	Х	98/137~(72%)	87 (89%)	7 (7%)	4 (4%)	3	23
17	Y	72/77~(94%)	61 (85%)	11 (15%)	0	100	100
18	Z	88/109 (81%)	85 (97%)	3 (3%)	0	100	100
19	Е	245/271~(90%)	187 (76%)	57 (23%)	1 (0%)	34	72
20	b	44/56~(79%)	35 (80%)	9 (20%)	0	100	100
21	с	49/65~(75%)	34 (69%)	15 (31%)	0	100	100
22	d	55/60~(92%)	47 (86%)	6 (11%)	2 (4%)	3	26
23	е	67/73~(92%)	50 (75%)	16 (24%)	1 (2%)	10	45
24	f	35/37~(95%)	30 (86%)	5 (14%)	0	100	100
25	F	210/221~(95%)	173 (82%)	37 (18%)	0	100	100
26	G	208/243~(86%)	166 (80%)	40 (19%)	2 (1%)	15	54
27	Н	173/220 (79%)	145 (84%)	27 (16%)	1 (1%)	25	64
28	Ι	171/182 (94%)	142 (83%)	27 (16%)	2 (1%)	13	50
29	J	51/155~(33%)	41 (80%)	9 (18%)	1 (2%)	7	39
30	g	41/142 (29%)	36 (88%)	5 (12%)	0	100	100
31	a	36/94~(38%)	26 (72%)	9 (25%)	1 (3%)	5	32
32	h	44/116 (38%)	31 (70%)	12 (27%)	1 (2%)	6	36
All	All	3218/4086 (79%)	2630 (82%)	538 (17%)	50 (2%)	13	43

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 $5~{\rm of}~50$ Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	L	107	HIS
6	N	143	LEU
6	N	147	ALA
6	Ν	154	LEU
6	Ν	155	PRO

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.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
4	L	125/165~(76%)	124 (99%)	1 (1%)	81	91
5	М	101/101 (100%)	101 (100%)	0	100	100
6	Ν	135/144 (94%)	126 (93%)	9~(7%)	16	48
7	О	107/108~(99%)	107 (100%)	0	100	100
8	Р	96/96~(100%)	96 (100%)	0	100	100
9	Q	99/100~(99%)	99 (100%)	0	100	100
10	R	104/135~(77%)	101 (97%)	3 (3%)	42	71
11	S	102/114 (90%)	102 (100%)	0	100	100
12	Т	129/174~(74%)	122 (95%)	7 (5%)	22	55
13	U	126/176~(72%)	125 (99%)	1 (1%)	81	91
14	V	81/103 (79%)	80 (99%)	1 (1%)	71	87
15	W	112/129~(87%)	109 (97%)	3 (3%)	44	73
16	Х	85/111 (77%)	74 (87%)	11 (13%)	4	22
17	Y	64/67~(96%)	61 (95%)	3(5%)	26	60
18	Ζ	83/97~(86%)	79~(95%)	4 (5%)	25	60
19	Е	195/216~(90%)	189 (97%)	6 (3%)	40	70
20	b	39/49~(80%)	39 (100%)	0	100	100
21	с	48/59~(81%)	47 (98%)	1 (2%)	53	79
22	d	47/49~(96%)	45 (96%)	2(4%)	29	62
23	е	59/62~(95%)	58 (98%)	1 (2%)	60	82
24	f	34/34~(100%)	34 (100%)	0	100	100
25	F	174/182~(96%)	170 (98%)	4 (2%)	50	77
26	G	176/205~(86%)	169 (96%)	7 (4%)	31	64
27	Н	148/183~(81%)	146 (99%)	2(1%)	67	85
28	Ι	$\overline{147/154} \ (96\%)$	147 (100%)	0	100	100
29	J	47/134 (35%)	46 (98%)	1 (2%)	53	79
30	g	$\overline{39/121}~(32\%)$	39 (100%)	0	100	100
31	a	33/83~(40%)	32 (97%)	1 (3%)	41	71
32	h	40/96~(42%)	40 (100%)	0	100	100

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



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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2775/3447~(80%)	2707~(98%)	68~(2%)	50 75

5 of 68 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
26	G	71	ASN
26	G	81	ARG
27	Н	188	GLN
15	W	173	ARG
15	W	170	THR

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such side chains are listed below:

Mol	Chain	Res	Type
15	W	68	HIS
26	G	93	GLN
18	Ζ	77	ASN
26	G	71	ASN
27	Н	90	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	А	2796/2810~(99%)	962~(34%)	106 (3%)
2	С	101/106~(95%)	45~(44%)	4 (3%)
3	В	116/121~(95%)	54 (46%)	5 (4%)
All	All	3013/3037~(99%)	1061~(35%)	115 (3%)

5 of 1061 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	А	7	С
1	А	13	А
1	А	22	G
1	А	27	А
1	А	32	U

 $5~{\rm of}~115$ RNA pucker outliers are listed below:



Mol	Chain	Res	Type
1	А	1334	U
3	В	7	G
1	А	1828	U
2	С	35	U
1	А	2536	А

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 (i)

This section contains visualisations of the EMDB entry EMD-9572. 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.

Orthogonal projections (i) 6.1

6.1.1Primary map



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

6.2Central slices (i)

6.2.1Primary map



X Index: 156

Y Index: 156



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: 120

Y Index: 186

Z Index: 166

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



The images above show the 3D surface view of the map at the recommended contour level 0.132. 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 (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 516 $\rm nm^3;$ this corresponds to an approximate mass of 466 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 0.286 ${\rm \AA^{-1}}$



8 Fourier-Shell correlation (i)

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-9572 and PDB model 5H1S. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.132 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



9.2 Q-score mapped to coordinate model (i)



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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.132).



9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.132) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7241	0.4530
А	0.7631	0.4510
В	0.8056	0.4300
С	0.8048	0.4520
E	0.6718	0.4930
F	0.6857	0.4970
G	0.6495	0.4640
Н	0.2816	0.3440
Ι	0.5668	0.4240
J	0.2110	0.3920
L	0.7252	0.5060
М	0.5963	0.4760
N	0.6777	0.4590
0	0.6464	0.4630
Р	0.7127	0.5020
Q	0.6235	0.4310
R	0.6104	0.4800
S	0.7362	0.4770
Т	0.6274	0.4750
U	0.6057	0.4530
V	0.5718	0.4870
W	0.5732	0.4400
Х	0.6438	0.4660
Y	0.6956	0.4980
Z	0.6041	0.4490
a	0.1017	0.2240
b	0.6793	0.4930
С	0.6150	0.4100
d	0.6817	0.5020
е	0.7362	0.5200
f	0.6840	0.4880
g	0.5575	0.4140
h	0.7255	0.4920



