

Apr 23, 2024 – 12:30 pm BST

PDB ID 7AQD : EMDB ID EMD-11864 : Title : Structure of the bacterial RQC complex (Translocating State) Authors : Filbeck, S.; Pfeffer, S. Deposited on 2020-10-21 : 3.10 Å(reported) Resolution : Based on initial models 5H3X, 5H3W, 3J9W :

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 (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:

EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

# 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 3.10 Å.

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



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM\ structures}\ (\#{ m Entries})$
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	Quality of chain	
1	R	570	29% 67% 5% • •	24%
2	А	2918	75%	23% •
3	В	112	67%	31% •
4	С	277	99%	
5	D	209	99%	
6	Е	207	99%	
7	F	179	9%	•••
8	G	179	<b>•</b> 97%	•••



Mol	Chain	Length	Quality of chain	
9	Ι	141	63% 94%	• 6%
10	J	145	97%	••
11	K	122	100%	
12	L	146	99%	
13	М	144	94%	
14	N	120	08%	
15	0	120		
10	0	120	100%	
16	Q	119	97%	••
17	S	113	96%	·
18	Т	76	34% 39% 22%	•
19	U	103	97%	•
20	V	94	87%	13%
21	W	7	100%	
22	Х	62	90%	• 6%
23	Z	59	98%	
24	a	115	99%	
25	b	59	92%	8%
26	с	49	98%	
27	d	44	98%	
28	е	66	97%	
29	f	37	97%	
30	or	102	00%	
00	5	05	9970	
31	h	95	98%	•
32	i	66	97%	••



# 2 Entry composition (i)

There are 32 unique types of molecules in this entry. The entry contains 94357 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 protein called Rqc2 homolog RqcH.

Mol	Chain	Residues		At	AltConf	Trace			
1	R	433	Total 3519	C 2239	N 612	O 658	S 10	0	0

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

Mol	Chain	Residues			AltConf	Trace			
2	А	2918	Total 62663	C 27955	N 11572	O 20218	Р 2918	0	0

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

Mol	Chain	Residues		A	AltConf	Trace			
3	В	112	Total 2395	C 1068	N 435	O 780	Р 112	0	0

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

Mol	Chain	Residues		At		AltConf	Trace		
4	С	275	Total 2111	C 1312	N 416	0 377	S 6	0	0

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
5	D	207	Total 1575	C 988	N 290	O 292	${f S}{5}$	0	0

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

Mol	Chain	Residues		At	oms			AltConf	Trace
6	Е	205	Total 1561	C 980	N 289	O 290	${ m S} { m 2}$	0	0



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

Mol	Chain	Residues		At	oms	AltConf	Trace		
7	F	178	Total 1404	C 893	N 245	O 259	${ m S} 7$	0	0

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
8	G	175	Total 1342	C 835	N 248	O 257	${ m S} { m 2}$	0	0

• Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues		At	oms	AltConf	Trace		
9	Ι	133	Total 981	C 617	N 173	0 185	S 6	0	0

• Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues		At	$\mathbf{oms}$			AltConf	Trace
10	J	142	Total 1123	C 710	N 206	O 202	${S \atop 5}$	0	0

• Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues		At	oms			AltConf	Trace
11	K	122	Total 920	C 571	N 173	0 172	${S \atop 4}$	0	0

• Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues		At	$\mathbf{oms}$	AltConf	Trace		
12	L	146	Total 1081	C 671	N 207	O 201	${ m S} { m 2}$	0	0

• Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues		At	oms			AltConf	Trace
13	М	138	Total 1097	C 703	N 208	0 181	${S \atop 5}$	0	0

• Molecule 14 is a protein called 50S ribosomal protein L17.



Mol	Chain	Residues		At	oms			AltConf	Trace
14	N	119	Total 953	C 583	N 186	O 180	$\frac{S}{4}$	0	0

• Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues		At	oms	AltConf	Trace		
15	0	120	Total 912	C 564	N 176	0 171	S 1	0	0

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
16	Q	117	Total 940	C 591	N 189	0 156	$\frac{S}{4}$	0	0

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

Mol	Chain	Residues		At	$\mathbf{oms}$	AltConf	Trace		
17	S	109	Total 842	C 525	N 164	O 150	${ m S} { m 3}$	0	0

• Molecule 18 is a RNA chain called Ala-tRNA (A/P-site).

Mol	Chain	Residues		$\mathbf{A}$	toms			AltConf	Trace
18	Т	76	Total 1622	C 722	N 290	0 534	Р 76	0	0

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
19	U	100	Total 754	C 473	N 141	0 137	${ m S} { m 3}$	0	0

• Molecule 20 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues		Ato	ms		AltConf	Trace
20	V	82	Total 630	C 390	N 123	0 117	0	0

• Molecule 21 is a protein called nascent polyalanine.



Mol	Chain	Residues	A	Aton	ns	AltConf	Trace	
21	W	7	Total	С	Ν	0	0	0
		•	35	21	7	7		

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

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
22	Х	58	Total 444	C 275	N 92	O 75	${ m S} { m 2}$	0	0

• Molecule 23 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
23	Ζ	58	Total 455	C 281	N 89	0 84	S 1	0	0

• Molecule 24 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
24	a	114	Total 936	C 595	N 184	0 157	0	0

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

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
25	b	54	Total 426	C 262	N 86	0 71	S 7	0	0

• Molecule 26 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
26	0	48	Total	С	Ν	Ο	S	0	0
20	C	40	401	244	80	73	4	0	0

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

Mol	Chain	Residues		Atc	$\mathbf{ms}$	AltConf	Trace		
27	d	44	Total 367	C 222	N 89	O 54	${S \over 2}$	0	0

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



Mol	Chain	Residues		Ate	oms	AltConf	Trace		
28	е	64	Total 512	C 321	N 107	O 82	${ m S} { m 2}$	0	0

• Molecule 29 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
29	f	36	Total 288	C 181	N 59	0 44	${S \over 4}$	0	0

 $\bullet\,$  Molecule 30 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
30	g	101	Total 786	C 501	N 139	O 146	0	0

• Molecule 31 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues		At	AltConf	Trace			
31	h	93	Total 752	C 472	N 137	O 139	${S \atop 4}$	0	0

• Molecule 32 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues		At	oms	AltConf	Trace		
32	i	65	Total 530	C 328	N 102	O 98	${S \over 2}$	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: Rqc2 homolog RqcH



(2382) (2383) (2383) (2383) (2383) (2394) (2394) (2395) (2394) (2395) (2394) (2395) (2394) (2395) (2394) (2	U300 U300 U300 U300 U310 U311 U312 U312 U312 U312 U322 U322	A325 A325 A337 A337 A345 A345 C346 C346 C352 A355 A355 A355 A355	C360 C367 C367 A374 A376 A376 C376 C376 C376 C376 C376 C376 C376 C
U386 C387 C387 C387 C382 C392 U394 U394 C392 C392 C392 C410 C411 C411 C411 C411	0413 0414 0417 0417 0417 0430 0432 0432 0433 0433 0435 0435 0435 0435 0435 0435	4438 6442 6444 6444 6444 6444 6444 0444 0444	4490 4494 1498 1498 1498 1502 1503 1504 1504 1514
6528 4537 4537 4537 4549 6550 6550 6551 6552 0556 7555 0555 0555	6568 C562 C563 C564 C570 C570 C570 C570 A571 A577 A578 C588 C588	A 592 A 593 A 593 A 595 A 595 A 617 A 618 A 618 A 618 A 618 A 618 A 613 A 613 A 613 A 647 C 644	0650 0651 0651 0660 0662 0665 0665 0665 0665 0665 0665
G650 G650 G684 G684 G684 U691 U700 G713 U714 A715 A715 C716	07118 07118 0719 0719 0773 0773 0777 0777 0777 0777	C785 A786 C792 C793 U794 C795 A795 A795 C394 C6324 C6324 C6324	4830 1831 6832 6833 886 6838 6838 6853 6853 6853 6853
A866 1874 1875 1876 1876 1876 1876 1893 1893 1893 1893 1893 1893 1893 1893	A913 C914 U924 A925 A925 C931 C931 A935 C935 C935 C937	U942 4943 4943 4945 4948 4948 4951 0953 0953 0953 0954 0955 0955 0955	U960 C961 C963 C963 C963 C964 A964 A973 A977 A977 A977 C980 C980 C981
A987 (2988 (2998 (2999 (2999 (2990 (2992) (2992) (2992) (2992) (2992) (2992) (21007 (21007) (2107) (21	A1025 A1026 A1027 C1028 A1029 C1031 A1034 A1034 A1058 U1058	A1059 G1068 U1068 A1072 A1072 A1092 A1093 A1093 G1093 C1095	A11102 A11104 U11104 U11106 U11106 G1109 G11109 U11111 U11111 U11111 U11112 A11112 A11112 A11113
A1116 G1117 C1128 A1128 U1127 U1128 U1128 U1128 A1130 G1136 G1135	G1139 U1440 A1141 A1144 A1144 A1144 A1144 A1148 G1152 A1157 G1158 G1158 G1158	U1176 U1177 U1178 U1179 C1180 C1180 C1180 C1186 C1186 U1187 A1194 A121	A1202 61209 01217 01218 61220 01229 01229 01246 61246 61246 61246
61250 01251 01255 01276 01276 01276 01278 01278 01278	A1293 A1295 01295 01295 01295 01295 01295 01315 01327 01337 01327 01337 01370000000000	A1340 U1345 A1346 A1346 U1351 U1353 C1353 C1363 C1363 C1363 C1363	A1381 A1382 C1384 C1384 A1388 A1388 A1388 A1417
U1418 A1423 A1423 A1425 C1425 C1425 G1431 A1432 A1432 A1435 U1436 C1437 C1437 C1438 U1439	U1440 U1441 A1442 C1450 A1456 A1456 A1473 C1474 C1474 C1474	A1490 C1499 C1499 A1499 U1607 U1613 C1513 C1513 C1515 C1519 A1520 A1520	uls28 ♦ 11528 ♦ 11536 11544 11559 11564 11553
A1555 41555 41562 41563 41563 41569 41571 41571 41571 41571 41572 41572	41583 01584 01584 01586 01586 01596 01596 01596 01596 01596 01596 01596 01596 01596 01596 01596 01596 01596 01596 01596 01596 01596 01584 01584 01584 01584 01584 01584 01584 01584 01584 01584 01584 01584 01584 015888 01588 01588 01588 01588 01588 01588 01588 01588 01588 01588 01588 01588 01588 015888 015888 010000000000	C1622 U1626 01630 01633 01633 01633 01633 01635 01655 01655 01655 01655 01655	11658 11659 11660 11667 11674 11674 11692 11692 11692
G1696 A1697 C1705 C1705 G1712 G1719 A1727 A1727 A1745	G1752 C1755 C1755 C1756 C1756 C1775 C1771 C1771 A1774 A1774 A1778 A1778	C1780 C1780 C1781 G1783 G1783 G1785 G1785 G1785 G1785 G1792 G1792 C1794 C1802 C1802	U1804 G1805 G1805 G1809 G1810 C1811 C1810 G1830 G1830 G1830 A1845 A1845 A1858
C1859 A1877 A1877 A1881 A1895 G1898 G1898 A1901 G1902 G1912 A1913	U1916 01917 01918 01928 01935 01935 01935 01935 01937 01949 01948 01948 01948	(1968 (1963 (1963 (1966 (1966 (1966 (1966 (1966 (1966 (1971 (1972 (1972 (1972 (1972) (1985	C1990 C1993 C1996 C1996 A1999 A2000 C1996 A2010 V2011
U2020 C2021 U2022 U2023 C2023 C2025 C2025 C2035 C2035 C2035 A2050 C2055 A2050	42061 42062 62068 62068 72084 72084 72088 72088 72088 72089 62090 62092 72092	C2110 C2110 A3111 C2122 A3123 A2123 A2123 A2121 C2133 A2141 C2142 C2142	A2143 A2144 C2145 C2145 C2146 C2149 A2149 C2149 C2149 C2155 C2155 C2151 C2151 C2151 C2151
(2162 A2165 A2165 C2175 A2176 A2176 A2176 A2187 A2187 A2187 C2183 C2193	(2195 12196 (2197 (2197 (2198 (2198 (2198 (2233 (2233 (2233 (2233 (2235) (2234) (2235) (2225) (225) (2255) (2255) (2255) (2255) (2255) (2255) (2255) (2255) (2255) (2255) (2255) (2255) (2255) (2255) (2255) (2255) (2255) (2255) (2255) (2255)	C22.43 C22.43 A2255 C22555 C22555 C2268 C2268 C2283 C2283 C2283 C2283 C2283 C2283 C2283 C2283	22311 22312 A2315 A2315 A2315 A2316 A2316 A2316 C2323 C2323 C2336 C2336 C2336 C2336 C2336 C2336 C2336 C2336 C2338 C2337 C2338 C2312 C2312 C2312 C2312 C2312 C2312 C2312 C2312 C2312 C2312 C2312 C2312 C2312 C2312 C2312 C2312 C2315 C2315 C2315 C2315 C2315 C2323 C2323 C2323 C2323 C2323 C2323 C2323 C2323 C2323 C2323 C2323 C2323 C2323 C2323 C2323 C2233 C2

WORLDWIDE PROTEIN DATA BANK



Chain G:	97%		
MET S2 S13 S13 D14 L72 K176 K176 SER ALA LYS			
• Molecule 9: 50S ribose	omal protein L11		
Chain I:	63% 94%	• 6%	
MET ALA LYS LYS LYS VAL VAL LYS V9 V9 V9 A15 C15 C15 C15 C15 C15 C15 C15 C15 C15 C	N19 P20 P23 P23 P23 P24 P25 P25 P25 P25 P25 P25 P25 P25 P25 P25	F 38 F 44 F 44 F 44 F 42 A 47 A 45 A 45	D63
R64 S65 F66 T67 F68 F68 T69 T70 K71 T72 P73 P73 P73 C84 C84 N93	R94 N95 V97 A98 A98 A98 A100 K101 R102 K102 D103 E103 A109 E110 T111 T111 T111 M113	P114 D115 L116 A118 A118 A119 D120 V121 E122 E122 H125 V128 T126 V138 E140 ASP	
• Molecule 10: 50S ribo	somal protein L13		
Chain J:	97%		
MET ARG THR T4 C2 G145 G145			
• Molecule 11: 50S ribo	somal protein L14		
Chain K:	100%		
There are no outlier res	idues recorded for this chain.		
• Molecule 12: 50S ribo	somal protein L15		
Chain L:	99%	·	
M1 N7 0 M86 M86 M116 1146			
• Molecule 13: 50S ribo	somal protein L16		
Chain M:	94%		
M1 R45 R60 C133 C133 C133 C133 C133 C133 C133 C13			
• Molecule 14: 50S ribo	somal protein L17		
Chain N:	98%	••	







• Molecule 21: nascent polya	lanine	
Chain W:	100%	
There are no outlier residues	recorded for this chain.	
• Molecule 22: 50S ribosoma	l protein L28	
Chain X:	90%	• 6%
MET ALA R3 R5 R56 V56 V56 V56 V56 V56 V56 V56 VAL		
• Molecule 23: 50S ribosoma	l protein L30	
Chain Z:	98%	
MET A2 q59		
• Molecule 24: 50S ribosoma	l protein L19	
Chain a:	99%	
MET 05 1112 K114 R116 R116		
• Molecule 25: 50S ribosoma	l protein L32	
Chain b:	92%	8%
MET A2 VAL LYS SER ASN		
• Molecule 26: 50S ribosoma	l protein L33 1	
Chain c:	98%	
M1 148 LYS		
• Molecule 27: 50S ribosoma	l protein L34	
Chain d:	98%	·
M1 K25 A44		

• Molecule 28: 50S ribosomal protein L35



Chain e:	97% .	
MET P2 LYS LYS		
• Molecule 29	50S ribosomal protein L36	
Chain f:	97% •	
MET K2 G37		
• Molecule 30	50S ribosomal protein L21	
Chain g:	99%	
MET Y2 T52 A102		
• Molecule 31	50S ribosomal protein L23	
Chain h:	98% .	
M1 F93 GLU ALA		
• Molecule 32	50S ribosomal protein L29	
Chain i:	97%	
M1 R7 L37 N65 LYS		



# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24348	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.177	Depositor
Minimum map value	-0.071	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0085	Depositor
Map size (Å)	410.88, 410.88, 410.88	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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	B	ond lengths	Bond angles	
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	R	0.84	18/3590~(0.5%)	3.03	68/4835~(1.4%)
2	А	0.34	1/70190~(0.0%)	1.05	279/109503~(0.3%)
3	В	0.32	0/2678	1.10	19/4174~(0.5%)
4	С	0.27	0/2148	0.54	0/2881
5	D	0.28	0/1597	0.55	1/2140~(0.0%)
6	Е	0.28	0/1580	0.56	0/2132
7	F	0.30	0/1423	0.65	1/1910~(0.1%)
8	G	0.29	0/1360	0.56	1/1832~(0.1%)
9	Ι	0.29	0/995	0.59	0/1346
10	J	0.30	0/1146	0.60	1/1542~(0.1%)
11	Κ	0.28	0/927	0.58	0/1245
12	L	0.29	0/1093	0.52	0/1457
13	М	0.34	0/1120	0.63	3/1496~(0.2%)
14	Ν	0.26	0/960	0.51	1/1284~(0.1%)
15	0	0.27	0/921	0.58	0/1236
16	Q	0.28	0/952	0.54	1/1266~(0.1%)
17	S	0.27	0/851	0.57	0/1146
18	Т	1.13	1/1811~(0.1%)	1.90	74/2822~(2.6%)
19	U	0.27	0/764	0.53	0/1022
20	V	0.32	0/638	0.59	0/847
21	W	0.31	0/34	0.86	0/46
22	Х	0.28	0/448	0.68	1/596~(0.2%)
23	Ζ	0.28	0/457	0.54	0/613
24	a	0.25	0/949	0.51	0/1269
25	b	0.29	0/433	0.61	0/574
26	с	0.27	0/406	0.53	0/540
27	d	0.24	0/370	0.45	0/483
28	е	0.28	0/519	0.55	0/680
29	f	0.24	0/291	0.44	0/383
30	g	0.30	0/797	0.66	0/1070
31	h	0.26	0/759	0.49	0/1011
32	i	0.28	0/531	0.65	1/707~(0.1%)
All	All	0.38	20/102738~(0.0%)	1.11	451/154088~(0.3%)



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
1	R	0	15
2	А	0	7
4	С	0	1
9	Ι	0	1
18	Т	0	14
All	All	0	38

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	430	LYS	CA-CB	14.59	1.86	1.53
1	R	429	GLY	C-N	13.71	1.65	1.34
1	R	3	PHE	CB-CG	11.71	1.71	1.51
1	R	3	PHE	CG-CD1	9.22	1.52	1.38
18	Т	72	С	C4-N4	-8.93	1.25	1.33
1	R	431	TYR	CB-CG	-8.80	1.38	1.51
1	R	431	TYR	CE2-CZ	-8.72	1.27	1.38
1	R	431	TYR	C-O	-8.34	1.07	1.23
1	R	431	TYR	C-N	7.99	1.52	1.34
1	R	412	SER	C-N	7.59	1.51	1.34
1	R	434	PRO	CA-CB	7.15	1.67	1.53
1	R	431	TYR	CD1-CE1	6.96	1.49	1.39
1	R	415	SER	C-N	6.88	1.47	1.34
1	R	4	ASP	N-CA	6.86	1.60	1.46
1	R	433	ARG	C-N	-5.67	1.23	1.34
1	R	434	PRO	CA-C	5.50	1.63	1.52
1	R	434	PRO	N-CD	-5.48	1.40	1.47
2	А	2010	А	N9-C4	5.13	1.41	1.37
1	R	433	ARG	CA-CB	-5.03	1.42	1.53
1	R	431	TYR	CZ-OH	5.02	1.46	1.37

in (101) sond angle outliers are instea seron.	All (	(451)	bond	angle	outliers	are	listed	below:
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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	R	431	TYR	CD1-CG-CD2	-78.07	32.02	117.90
1	R	431	TYR	CG-CD2-CE2	-71.48	64.12	121.30
1	R	3	PHE	CD1-CE1-CZ	-71.22	34.63	120.10
1	R	431	TYR	CG-CD1-CE1	-71.09	64.43	121.30



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Mol	Chain	$\operatorname{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	R	3	PHE	CB-CG-CD1	58.90	162.03	120.80
1	R	3	PHE	CG-CD1-CE1	-57.69	57.34	120.80
1	R	3	PHE	CD1-CG-CD2	-40.51	65.63	118.30
1	R	430	LYS	N-CA-CB	-39.03	40.35	110.60
1	R	3	PHE	CZ-CE2-CD2	-37.46	75.15	120.10
1	R	3	PHE	CG-CD2-CE2	-34.79	82.53	120.80
1	R	3	PHE	CE1-CZ-CE2	-32.96	60.68	120.00
1	R	431	TYR	CB-CG-CD1	-29.58	103.25	121.00
1	R	431	TYR	CZ-CE2-CD2	-25.08	97.23	119.80
1	R	431	TYR	CE1-CZ-CE2	-23.90	81.56	119.80
1	R	429	GLY	C-N-CA	-20.51	70.44	121.70
1	R	431	TYR	CB-CG-CD2	18.53	132.12	121.00
1	R	431	TYR	N-CA-CB	-16.81	80.34	110.60
1	R	433	ARG	C-N-CD	-14.99	87.62	120.60
1	R	414	ALA	CB-CA-C	-14.89	87.77	110.10
1	R	2	SER	C-N-CA	-13.85	87.08	121.70
1	R	431	TYR	CE1-CZ-OH	11.89	152.20	120.10
1	R	433	ARG	CB-CG-CD	-11.24	82.38	111.60
2	А	2511	A	N1-C6-N6	-10.95	112.03	118.60
1	R	351	TYR	CG-CD1-CE1	-10.90	112.58	121.30
1	R	3	PHE	N-CA-CB	10.89	130.20	110.60
1	R	3	PHE	CB-CG-CD2	10.85	128.39	120.80
2	А	2479	A	N1-C6-N6	-10.38	112.37	118.60
18	Т	76	A	N1-C6-N6	-10.18	112.49	118.60
18	Т	21	A	N1-C6-N6	-10.17	112.50	118.60
2	А	2489	U	O4'-C1'-N1	10.11	116.28	108.20
1	R	415	SER	CB-CA-C	-9.98	91.13	110.10
1	R	351	TYR	CD1-CE1-CZ	9.84	128.65	119.80
18	Т	14	A	N1-C6-N6	-9.81	112.71	118.60
1	R	3	PHE	CA-C-O	-9.79	99.54	120.10
2	A	2631	A	N1-C6-N6	-9.67	112.80	118.60
2	A	272	С	C2-N1-C1'	9.62	129.38	118.80
2	A	1281	С	N1-C2-O2	9.55	124.63	118.90
2	A	483	С	C2-N1-C1'	9.39	129.13	118.80
2	A	1352	U	C2-N1-C1'	9.36	128.94	117.70
2	A	914	C	N1-C2-O2	9.35	124.51	118.90
1	R	430	LYS	C-N-CA	9.35	145.06	121.70
2	A	2480	A	N1-C6-N6	-9.28	113.03	118.60
2	A	1657	C	C5-C6-N1	9.23	125.61	121.00
2	A	1281	C	N3-C2-O2	-9.20	115.46	121.90
1	R	3	PHE	CA-C-N	9.17	137.38	117.20
1	R	433	ARG	CB-CA-C	-9.13	92.15	110.40



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	1352	U	N1-C2-O2	9.00	129.10	122.80
1	R	3	PHE	CB-CA-C	-8.98	92.44	110.40
1	R	413	SER	C-N-CA	8.93	144.03	121.70
2	А	1564	С	N1-C2-O2	8.87	124.22	118.90
2	А	1352	U	N3-C2-O2	-8.83	116.02	122.20
2	А	2488	А	P-O3'-C3'	8.83	130.29	119.70
2	А	2712	С	N1-C2-O2	8.77	124.16	118.90
2	А	2480	А	C5-C6-N1	8.66	122.03	117.70
2	А	1281	С	C2-N1-C1'	8.62	128.28	118.80
1	R	4	ASP	CB-CG-OD1	-8.61	110.56	118.30
18	Т	66	A	N1-C6-N6	-8.56	113.46	118.60
1	R	279	PHE	CD1-CE1-CZ	8.55	130.36	120.10
2	А	1246	G	O4'-C1'-N9	8.44	114.95	108.20
1	R	279	PHE	CG-CD1-CE1	-8.29	111.69	120.80
1	R	430	LYS	CB-CG-CD	8.24	133.03	111.60
18	Т	9	A	N1-C6-N6	-8.23	113.67	118.60
1	R	434	PRO	N-CA-CB	-8.19	93.48	103.30
18	Т	23	A	C5-C6-N1	8.09	121.75	117.70
2	А	716	G	C4-N9-C1'	7.99	136.88	126.50
2	А	914	C	C2-N1-C1'	7.94	127.53	118.80
18	Т	44	A	C5-C6-N1	7.88	121.64	117.70
1	R	430	LYS	CD-CE-NZ	-7.87	93.59	111.70
18	Т	62	C	N3-C2-O2	-7.86	116.40	121.90
18	Т	44	A	N1-C6-N6	-7.86	113.89	118.60
3	В	28	С	N1-C2-O2	7.84	123.60	118.90
2	А	1281	С	C6-N1-C2	-7.80	117.18	120.30
2	А	442	С	C2-N1-C1'	7.79	127.37	118.80
2	А	1622	С	C2-N1-C1'	7.78	127.36	118.80
2	А	2489	U	N3-C2-O2	-7.72	116.80	122.20
1	R	3	PHE	C-N-CA	7.71	140.97	121.70
1	R	4	ASP	O-C-N	-7.69	110.12	123.20
2	A	203	U	C2-N1-C1'	7.67	126.90	117.70
2	А	203	U	N1-C2-O2	7.64	128.15	122.80
2	А	2712	С	C2-N1-C1'	7.61	127.17	118.80
13	М	45	ARG	NE-CZ-NH1	7.58	124.09	120.30
18	Т	66	A	C5-C6-N1	7.57	121.49	117.70
7	F	83	MET	CA-CB-CG	7.54	126.11	113.30
18	Т	69	C	N3-C2-O2	-7.50	116.65	121.90
2	A	1564	C	N3-C2-O2	-7.49	116.66	121.90
2	А	914	C	N3-C2-O2	-7.46	116.68	121.90
1	R	433	ARG	CA-C-N	-7.44	96.28	117.10
2	А	2480	A	C4-C5-C6	-7.38	113.31	117.00



 $Ideal(^{o})$ 

120.30 108.20 121.90 120.30 108.20 118.80 108.20 117.70 122.80 118.30119.70 108.20 122.20 117.70 121.90 117.70 118.90 108.20 118.90 118.80 117.70 110.60 118.80 117.00 121.90 118.90126.00 128.60 118.80 106.50121.90 119.70 119.70 118.90

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$
2	А	483	С	C6-N1-C2	-7.36	117.36
2	А	1345	U	O4'-C1'-N1	7.33	114.07
18	Т	11	С	N3-C2-O2	-7.33	116.77
2	А	272	С	C6-N1-C2	-7.31	117.38
2	А	2376	С	O4'-C1'-N1	7.30	114.04
2	А	1515	С	C2-N1-C1'	7.29	126.82
18	Т	22	G	O4'-C1'-N9	7.26	114.00
2	А	2631	А	C5-C6-N1	7.23	121.31
2	А	237	U	N1-C2-O2	7.15	127.81
1	R	4	ASP	CB-CG-OD2	7.14	124.73
2	А	2785	U	P-O3'-C3'	7.14	128.27
18	Т	48	С	O4'-C1'-N1	7.14	113.91
2	А	203	U	N3-C2-O2	-7.13	117.20
18	Т	9	А	C5-C6-N1	7.13	121.27
18	Т	64	С	N3-C2-O2	-7.12	116.91
18	Т	76	А	C5-C6-N1	7.12	121.26
2	А	1544	С	N1-C2-O2	7.12	123.17
2	А	1696	G	O4'-C1'-N9	7.09	113.87
2	А	1550	С	N1-C2-O2	7.08	123.15
2	А	1963	С	C2-N1-C1'	7.08	126.59
18	Т	14	А	C5-C6-N1	7.07	121.24
2	А	2010	А	C2-N3-C4	7.07	114.14
2	А	234	С	C2-N1-C1'	7.03	126.53
18	Т	14	А	C4-C5-C6	-7.00	113.50
18	Т	6	С	N3-C2-O2	-7.00	117.00
2	А	1515	С	N1-C2-O2	6.99	123.09
2	А	716	G	N3-C4-N9	6.98	130.19
2	А	716	G	N3-C4-C5	-6.93	125.14
2	А	1564	С	C2-N1-C1'	6.92	126.41
1	R	434	PRO	CB-CG-CD	-6.92	79.53
2	А	2093	С	N3-C2-O2	-6.90	117.07
2	А	1245	G	P-O3'-C3'	6.88	127.96
2	A	377	G	P-O3'-C3'	6.88	127.95
2	А	2255	С	N1-C2-O2	6.85	123.01

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18

С

ASP

TYR

С

G

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С

U

O4'-C1'-N1

CA-C-N

CB-CG-CD1

C2'-C3'-O3'

C8-N9-C1'

C6-N1-C2

N3-C2-O2

O4'-C1'-N1

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716

1657

2712

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121.00

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121.90

108.20

113.68

129.84

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124.61

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117.59

117.16

113.62



6.85

6.82

-6.82

6.82

-6.80

-6.78

-6.77

6.77

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	1110	С	C2-N1-C1'	6.75	126.23	118.80
2	А	2459	A	C2-N3-C4	6.75	113.97	110.60
2	А	936	С	P-O3'-C3'	6.74	127.79	119.70
2	А	1028	С	N1-C2-O2	6.72	122.93	118.90
18	Т	13	С	N3-C4-N4	-6.72	113.29	118.00
2	А	1351	U	P-O3'-C3'	6.71	127.75	119.70
18	Т	66	А	C4-C5-C6	-6.68	113.66	117.00
2	А	2568	С	C2-N1-C1'	6.67	126.14	118.80
2	А	1229	U	N1-C2-O2	6.66	127.47	122.80
2	А	1803	С	C6-N1-C2	-6.66	117.64	120.30
18	Т	71	С	N3-C2-O2	-6.66	117.24	121.90
2	А	683	А	P-O3'-C3'	6.65	127.68	119.70
2	А	1362	G	P-O3'-C3'	6.64	127.67	119.70
2	А	1652	С	P-O3'-C3'	6.63	127.66	119.70
2	А	1985	U	N1-C2-O2	6.63	127.44	122.80
2	А	237	U	N3-C2-O2	-6.62	117.56	122.20
2	А	483	С	C5-C6-N1	6.61	124.31	121.00
2	А	188	С	C5-C6-N1	6.61	124.30	121.00
18	Т	25	С	N3-C2-O2	-6.61	117.28	121.90
18	Т	11	С	N1-C2-O2	6.61	122.86	118.90
2	А	1803	С	N1-C2-O2	6.57	122.84	118.90
2	А	1110	С	N1-C2-O2	6.56	122.84	118.90
18	Т	13	С	N3-C2-O2	-6.54	117.32	121.90
2	А	113	U	C2-N1-C1'	6.54	125.54	117.70
2	А	1353	С	C2-N1-C1'	6.53	125.98	118.80
2	А	484	С	C2-N1-C1'	6.53	125.98	118.80
2	А	2479	А	C4-C5-C6	-6.52	113.74	117.00
18	Т	44	А	C5'-C4'-C3'	-6.52	105.57	116.00
18	Т	76	A	C4-C5-C6	-6.50	113.75	117.00
2	А	914	C	C6-N1-C2	-6.50	117.70	120.30
2	А	1245	G	O4'-C1'-N9	6.49	113.39	108.20
1	R	433	ARG	N-CA-C	6.49	128.53	111.00
18	Т	44	А	C5'-C4'-O4'	6.49	116.89	109.10
3	В	28	С	C2-N1-C1'	6.48	125.92	118.80
1	R	260	LEU	CA-CB-CG	6.46	130.17	115.30
2	A	1564	C	C6-N1-C2	-6.46	117.71	120.30
2	А	2503	С	C2-N1-C1'	6.46	125.91	118.80
2	A	1771	C	C2-N1-C1'	6.46	125.90	118.80
18	Т	23	A	N1-C6-N6	-6.44	114.73	118.60
2	А	195	С	N1-C2-O2	6.44	122.76	118.90
1	R	277	PHE	CB-CG-CD1	-6.40	116.32	120.80
1	R	430	LYS	N-CA-C	-6.40	93.72	111.00



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	272	С	C6-N1-C1'	-6.39	113.14	120.80
2	А	272	С	N1-C2-O2	6.38	122.73	118.90
2	А	1970	С	N1-C2-O2	6.38	122.73	118.90
2	А	717	A	P-O3'-C3'	6.38	127.35	119.70
18	Т	51	С	N3-C2-O2	-6.37	117.44	121.90
18	Т	62	С	N1-C2-O2	6.37	122.72	118.90
14	N	83	LEU	CA-CB-CG	6.34	129.88	115.30
2	А	104	С	C2-N1-C1'	6.33	125.76	118.80
2	А	2511	A	C5-C6-N1	6.33	120.86	117.70
2	А	483	C	N1-C2-O2	6.30	122.68	118.90
3	В	28	С	N3-C2-O2	-6.29	117.50	121.90
18	Т	21	A	C4-C5-C6	-6.28	113.86	117.00
2	А	1970	C	C2-N1-C1'	6.25	125.67	118.80
2	А	1985	U	N3-C2-O2	-6.24	117.83	122.20
3	В	79	C	N1-C2-O2	6.22	122.63	118.90
18	Т	7	U	C3'-C2'-C1'	6.22	106.48	101.50
18	Т	7	U	O4'-C1'-N1	6.22	113.17	108.20
2	А	2512	C	N3-C2-O2	-6.21	117.55	121.90
2	А	1572	G	O4'-C1'-N9	6.20	113.16	108.20
2	А	188	C	C6-N1-C2	-6.18	117.83	120.30
2	А	1922	C	N3-C2-O2	-6.18	117.58	121.90
2	А	1803	С	N3-C2-O2	-6.17	117.58	121.90
1	R	412	SER	C-N-CA	-6.17	106.29	121.70
2	А	1922	C	N1-C2-O2	6.16	122.60	118.90
2	А	1411	U	N3-C2-O2	-6.16	117.89	122.20
2	А	261	C	N1-C2-O2	6.16	122.59	118.90
13	М	82	ARG	NE-CZ-NH1	6.15	123.38	120.30
2	А	2585	C	N1-C2-O2	6.14	122.58	118.90
2	А	1069	U	N1-C2-O2	6.14	127.10	122.80
3	В	35	C	N1-C2-O2	6.14	122.58	118.90
2	А	483	С	C6-N1-C1'	-6.13	113.44	120.80
2	А	2712	С	C6-N1-C2	-6.13	117.85	120.30
2	А	719	C	C2-N1-C1'	6.12	125.53	118.80
2	А	2468	A	P-O3'-C3'	6.11	127.04	119.70
2	А	2838	U	N3-C2-O2	-6.11	117.92	122.20
2	А	437	A	P-O3'-C3'	6.11	127.03	119.70
2	A	272	C	C5-C6-N1	6.06	124.03	121.00
18	Т	51	C	O4'-C1'-N1	6.06	113.05	108.20
1	R	351	TYR	CB-CG-CD1	-6.06	117.36	121.00
2	A	2511	A	C4-C5-C6	-6.06	113.97	117.00
2	A	$25\overline{2}$	C	N1-C2-O2	$6.0\overline{5}$	$122.5\overline{3}$	118.90
2	A	981	С	$C2-N1-\overline{C1'}$	6.05	125.45	118.80



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
18	Т	49	A	N1-C6-N6	-6.04	114.98	118.60
2	А	2072	С	C2-N1-C1'	6.03	125.44	118.80
18	Т	20	G	P-O3'-C3'	6.00	126.90	119.70
2	А	2631	A	O4'-C1'-N9	5.98	112.98	108.20
1	R	413	SER	CB-CA-C	-5.97	98.76	110.10
2	А	2648	U	N3-C2-O2	-5.96	118.03	122.20
2	А	588	С	C2-N1-C1'	5.95	125.34	118.80
2	А	90	А	P-O3'-C3'	5.95	126.84	119.70
2	А	1368	U	N3-C2-O2	-5.95	118.04	122.20
2	А	2839	С	N1-C2-O2	5.95	122.47	118.90
2	А	288	С	N3-C2-O2	-5.94	117.74	121.90
18	Т	72	С	N3-C2-O2	-5.94	117.74	121.90
2	А	1028	С	C2-N1-C1'	5.92	125.31	118.80
2	А	1963	С	C6-N1-C2	-5.91	117.93	120.30
3	В	91	С	C2-N1-C1'	5.91	125.30	118.80
3	В	45	С	N1-C2-O2	5.91	122.44	118.90
1	R	278	TYR	CB-CG-CD2	5.90	124.54	121.00
2	А	183	А	OP1-P-O3'	5.89	118.15	105.20
18	Т	22	G	N3-C2-N2	-5.88	115.78	119.90
2	А	1352	U	C6-N1-C1'	-5.87	112.98	121.20
2	А	1515	С	C6-N1-C2	-5.87	117.95	120.30
2	А	962	C	C2-N1-C1'	5.86	125.24	118.80
2	А	2796	С	P-O3'-C3'	5.85	126.72	119.70
2	А	1859	С	C5-C6-N1	5.84	123.92	121.00
2	А	77	U	C2-N1-C1'	5.84	124.71	117.70
2	А	979	U	N1-C2-O2	5.83	126.88	122.80
2	А	1859	C	C6-N1-C2	-5.83	117.97	120.30
2	А	2454	A	P-O3'-C3'	5.82	126.68	119.70
2	А	537	A	P-O3'-C3'	5.81	126.67	119.70
32	i	37	LEU	CA-CB-CG	5.81	128.66	115.30
2	A	945	С	N1-C2-O2	5.80	122.38	118.90
2	A	1794	C	C2-N1-C1'	5.80	125.18	118.80
2	A	1515	С	N3-C2-O2	-5.79	117.84	121.90
3	В	28	C	C6-N1-C2	-5.79	117.98	120.30
2	A	310	C	C2-N1-C1'	5.79	125.17	118.80
2	A	1544	С	N3-C2-O2	-5.79	117.85	121.90
2	A	1246	G	C4-N9-C1'	5.78	134.02	126.50
2	A	1755	C	P-O3'-C3'	5.78	126.63	119.70
3	В	24	C	N1-C2-O2	5.77	122.36	118.90
2	A	482	C	C2-N1-C1'	5.76	125.13	118.80
18	Т	21	A	C5-C6-N1	5.75	120.58	117.70
1	R	2	SER	CB-CA-C	5.75	121.03	110.10



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
18	Т	26	G	N1-C6-O6	-5.75	116.45	119.90
2	А	413	U	N3-C2-O2	-5.74	118.18	122.20
2	А	924	U	N1-C2-O2	5.74	126.82	122.80
18	Т	65	U	N3-C2-O2	-5.73	118.19	122.20
2	А	2022	U	N3-C2-O2	-5.73	118.19	122.20
2	А	1069	U	C2-N1-C1'	5.70	124.54	117.70
2	А	1916	U	N1-C2-O2	5.70	126.79	122.80
18	Т	44	А	C4-C5-C6	-5.69	114.15	117.00
2	А	1550	С	C2-N1-C1'	5.68	125.05	118.80
2	А	183	А	P-O3'-C3'	5.68	126.52	119.70
2	А	413	U	N1-C2-O2	5.68	126.78	122.80
2	А	549	А	P-O3'-C3'	5.67	126.51	119.70
3	В	19	G	C4-N9-C1'	5.67	133.87	126.50
2	А	104	С	N1-C2-O2	5.66	122.30	118.90
2	А	1437	С	C2-N1-C1'	5.66	125.02	118.80
18	Т	71	С	N1-C2-O2	5.65	122.29	118.90
1	R	280	GLY	O-C-N	5.65	131.74	122.70
2	А	2568	С	C6-N1-C2	-5.64	118.05	120.30
2	А	77	U	N1-C2-O2	5.63	126.74	122.80
18	Т	9	А	C4-C5-C6	-5.62	114.19	117.00
2	А	2503	С	N1-C2-O2	5.61	122.27	118.90
18	Т	65	U	O4'-C1'-N1	5.61	112.69	108.20
2	А	892	U	C2-N1-C1'	5.61	124.43	117.70
1	R	4	ASP	CA-CB-CG	-5.60	101.07	113.40
2	А	899	С	N3-C2-O2	-5.60	117.98	121.90
2	А	2351	А	P-O3'-C3'	5.60	126.42	119.70
2	А	2712	С	C5-C6-N1	5.60	123.80	121.00
2	А	1229	U	N3-C2-O2	-5.60	118.28	122.20
2	А	2781	С	N1-C2-O2	5.59	122.25	118.90
16	Q	94	MET	CA-CB-CG	5.58	122.79	113.30
2	А	1069	U	N3-C2-O2	-5.58	118.30	122.20
2	А	288	С	N1-C2-O2	5.57	122.24	118.90
18	Т	53	G	C4-N9-C1'	5.56	133.73	126.50
2	А	1031	С	C2-N1-C1'	5.56	124.91	118.80
2	А	2255	С	N3-C2-O2	-5.55	118.01	121.90
2	А	1368	U	C2-N1-C1'	5.55	124.36	117.70
2	А	1411	U	C2-N1-C1'	5.55	124.36	117.70
18	Т	71	С	O4'-C1'-N1	5.55	112.64	108.20
18	Т	49	А	C5-C6-N1	5.54	120.47	117.70
2	А	1438	С	P-O3'-C3'	5.54	126.35	119.70
2	А	442	С	C6-N1-C2	-5.54	118.09	120.30
18	Т	28	С	C2-N1-C1'	5.53	124.88	118.80



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	2685	U	N1-C2-O2	5.52	126.67	122.80
2	А	1691	A	C2-N3-C4	5.52	113.36	110.60
2	А	899	С	N1-C2-O2	5.51	122.21	118.90
2	А	2784	С	P-O3'-C3'	5.51	126.31	119.70
18	Т	5	С	N3-C2-O2	-5.50	118.05	121.90
2	А	2838	U	N1-C2-O2	5.50	126.65	122.80
1	R	432	LEU	C-N-CA	5.50	135.44	121.70
2	А	252	С	C2-N1-C1'	5.49	124.84	118.80
2	А	309	U	C2-N1-C1'	5.48	124.28	117.70
1	R	414	ALA	N-CA-C	5.47	125.78	111.00
2	А	234	С	N1-C2-O2	5.47	122.18	118.90
2	А	2072	C	C6-N1-C2	-5.47	118.11	120.30
2	А	1859	С	C2-N1-C1'	5.46	124.80	118.80
2	А	2010	А	N3-C4-C5	-5.45	122.99	126.80
2	А	2816	C	C2-N1-C1'	5.44	124.79	118.80
2	А	1622	С	C6-N1-C2	-5.42	118.13	120.30
8	G	72	LEU	CA-CB-CG	5.42	127.75	115.30
2	А	1803	С	C2-N1-C1'	5.41	124.76	118.80
1	R	432	LEU	CB-CA-C	-5.41	99.92	110.20
2	А	1916	U	N3-C2-O2	-5.41	118.41	122.20
18	Т	25	С	O4'-C1'-N1	5.41	112.53	108.20
2	A	2480	A	C6-C5-N7	5.40	136.08	132.30
18	Т	6	С	N1-C2-O2	5.40	122.14	118.90
18	Т	69	С	N1-C2-O2	5.39	122.13	118.90
2	A	662	U	P-O3'-C3'	5.38	126.16	119.70
2	А	195	С	C6-N1-C2	-5.37	118.15	120.30
3	В	35	С	N3-C2-O2	-5.37	118.14	121.90
2	A	2334	U	P-O3'-C3'	5.37	126.14	119.70
2	A	1622	С	N1-C2-O2	5.36	122.12	118.90
2	A	2283	С	O4'-C1'-N1	5.36	112.49	108.20
18	Т	48	С	N3-C2-O2	-5.36	118.15	121.90
2	A	1963	С	N1-C2-O2	5.36	122.11	118.90
18	Т	53	G	O4'-C1'-N9	5.36	112.49	108.20
2	A	924	U	N3-C2-O2	-5.35	118.45	122.20
2	A	924	U	C2-N1-C1'	5.34	124.11	117.70
2	A	442	C	C6-N1-C1'	-5.34	114.39	120.80
18	Т	62	C	N3-C4-N4	-5.34	114.27	118.00
2	A	2323	C	C2-N1-C1'	5.33	124.67	118.80
2	A	1622	C	C6-N1-C1'	-5.33	114.41	120.80
2	A	2489	U	C5'-C4'-C3'	-5.31	107.51	116.00
2	A	484	C	C6-N1-C2	-5.30	118.18	120.30
2	A	1916	U	C2-N1-C1'	5.30	124.06	117.70



Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
2	А	77	U	N3-C2-O2	-5.30	118.49	122.20
18	Т	60	С	C2-N1-C1'	5.29	124.62	118.80
2	А	252	С	C6-N1-C2	-5.29	118.18	120.30
2	А	2283	С	N3-C2-O2	-5.29	118.19	121.90
2	А	2839	С	N3-C2-O2	-5.29	118.20	121.90
2	А	229	А	P-O3'-C3'	5.29	126.04	119.70
2	А	1657	С	C2-N1-C1'	5.28	124.61	118.80
13	М	137	ILE	C-N-CA	5.28	133.38	122.30
1	R	412	SER	O-C-N	-5.27	114.27	122.70
3	В	19	G	OP1-P-O3'	5.26	116.78	105.20
2	А	1539	С	N1-C2-O2	5.26	122.06	118.90
2	А	2010	А	N3-C4-N9	5.25	131.60	127.40
2	А	1411	U	N1-C2-O2	5.25	126.47	122.80
2	А	413	U	C2-N1-C1'	5.25	123.99	117.70
18	Т	70	U	C3'-C2'-C1'	5.24	105.69	101.50
2	А	228	С	C6-N1-C2	-5.23	118.21	120.30
2	А	1353	С	N1-C2-O2	5.23	122.04	118.90
2	А	2513	G	C5'-C4'-C3'	-5.23	107.63	116.00
2	А	837	U	P-O3'-C3'	5.23	125.97	119.70
2	А	1281	С	C6-N1-C1'	-5.23	114.53	120.80
1	R	4	ASP	CB-CA-C	5.22	120.85	110.40
2	А	310	С	N1-C2-O2	5.22	122.03	118.90
18	Т	25	С	N1-C2-O2	5.22	122.03	118.90
2	А	2492	С	C2-N1-C1'	5.22	124.54	118.80
2	А	1352	U	C5-C6-N1	5.22	125.31	122.70
2	А	195	С	N3-C2-O2	-5.21	118.25	121.90
2	А	979	U	N3-C2-O2	-5.21	118.55	122.20
18	Т	26	G	C5-C6-N1	5.21	114.11	111.50
2	А	936	C	OP1-P-O3'	5.21	116.66	105.20
2	А	2632	G	N1-C6-O6	-5.21	116.78	119.90
2	А	1544	C	C6-N1-C2	-5.20	118.22	120.30
2	А	228	C	C2-N1-C1'	5.19	124.51	118.80
2	А	2631	A	C4-C5-C6	-5.19	114.41	117.00
1	R	433	ARG	NE-CZ-NH1	5.19	122.89	120.30
2	А	1544	C	C2-N1-C1'	5.19	124.50	118.80
2	A	$2\overline{479}$	A	C5-C6-N1	5.18	120.29	117.70
2	А	1937	C	N1-C2-O2	5.17	122.00	118.90
18	Т	15	G	N1-C6-O6	-5.17	116.80	119.90
2	A	1095	C	N1-C2-O2	5.16	122.00	118.90
2	A	1437	C	C6-N1-C2	-5.16	118.23	120.30
3	В	35	C	C6-N1-C2	-5.16	118.23	120.30
2	A	1229	U	C5-C6-N1	5.16	125.28	122.70



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Mol	Chain	$\operatorname{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	2337	G	N3-C4-C5	-5.16	126.02	128.60
1	R	337	TYR	CD1-CE1-CZ	-5.15	115.16	119.80
2	А	1937	С	C2-N1-C1'	5.15	124.47	118.80
2	А	158	С	C2-N1-C1'	5.15	124.46	118.80
2	А	1028	С	N3-C2-O2	-5.14	118.30	121.90
18	Т	72	С	C6-N1-C2	-5.14	118.24	120.30
2	А	831	U	N3-C2-O2	-5.14	118.60	122.20
2	А	1246	G	C8-N9-C1'	-5.14	120.32	127.00
2	А	1794	С	C6-N1-C2	-5.14	118.24	120.30
2	А	271	С	C2-N1-C1'	5.14	124.45	118.80
2	А	1550	С	N3-C2-O2	-5.14	118.30	121.90
1	R	279	PHE	CZ-CE2-CD2	-5.14	113.94	120.10
2	А	785	С	P-O3'-C3'	5.14	125.86	119.70
5	D	55	ASP	CB-CG-OD1	5.13	122.92	118.30
10	J	29	LEU	CA-CB-CG	5.13	127.11	115.30
3	В	79	С	N3-C2-O2	-5.13	118.31	121.90
2	А	159	U	N1-C2-O2	5.12	126.39	122.80
2	А	1691	А	C4-N9-C1'	5.12	135.52	126.30
2	А	1963	С	C5-C6-N1	5.12	123.56	121.00
2	А	2323	С	N1-C2-O2	5.12	121.97	118.90
2	А	2820	U	C2-N1-C1'	5.12	123.84	117.70
3	В	95	U	N1-C2-O2	5.12	126.38	122.80
1	R	431	TYR	CD1-CE1-CZ	-5.11	115.20	119.80
18	Т	70	U	N3-C2-O2	-5.11	118.62	122.20
2	А	309	U	N1-C2-O2	5.11	126.38	122.80
2	А	482	С	N1-C2-O2	5.10	121.96	118.90
2	А	1622	С	C5-C6-N1	5.10	123.55	121.00
2	А	2267	G	P-O3'-C3'	5.10	125.82	119.70
22	Х	23	ASN	C-N-CA	5.08	134.41	121.70
2	А	2632	G	C5-C6-N1	5.08	114.04	111.50
2	А	914	С	C6-N1-C1'	-5.08	114.71	120.80
2	А	1368	U	N1-C2-O2	5.08	126.35	122.80
2	А	2511	А	C6-C5-N7	5.07	135.85	132.30
2	А	1362	G	OP1-P-O3'	5.07	116.35	105.20
2	А	2035	С	C2-N1-C1'	5.07	124.38	118.80
18	Т	74	С	C4'-C3'-O3'	5.07	123.14	113.00
2	А	1333	С	C2-N1-C1'	5.07	124.37	118.80
2	A	2092	С	C2-N3-C4	-5.07	117.37	119.90
18	Т	51	C	N1-C2-O2	5.07	121.94	118.90
2	A	203	U	C5-C6-N1	5.06	125.23	122.70
2	A	2480	A	O4'-C1'-N9	5.06	112.25	108.20
18	Т	45	G	N3-C4-C5	-5.05	126.07	128.60



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	1970	С	N3-C2-O2	-5.05	118.36	121.90
3	В	19	G	P-O3'-C3'	5.05	125.76	119.70
2	А	570	С	C2-N1-C1'	5.05	124.36	118.80
2	А	1148	С	N1-C2-O2	5.05	121.93	118.90
2	А	405	U	P-O3'-C3'	5.04	125.75	119.70
3	В	19	G	C8-N9-C1'	-5.04	120.45	127.00
2	А	442	С	N1-C2-O2	5.04	121.92	118.90
2	А	898	U	N3-C2-O2	-5.04	118.67	122.20
2	А	1770	С	C2-N1-C1'	5.03	124.34	118.80
2	А	261	С	N3-C2-O2	-5.03	118.38	121.90
18	Т	72	С	C4'-C3'-C2'	-5.03	97.57	102.60
2	А	1948	А	P-O3'-C3'	5.03	125.73	119.70
2	А	159	U	N3-C2-O2	-5.02	118.68	122.20
1	R	434	PRO	CA-CB-CG	-5.02	94.46	104.00
2	А	1281	С	O4'-C1'-N1	5.02	112.22	108.20
3	В	95	U	C2-N1-C1'	5.02	123.72	117.70
3	В	19	G	N3-C4-N9	5.02	129.01	126.00
2	А	422	С	C2-N1-C1'	5.01	124.32	118.80
2	А	2092	С	O4'-C1'-N1	5.01	112.21	108.20
2	А	2110	С	C2-N1-C1'	5.01	124.31	118.80
18	Т	12	U	N3-C2-O2	-5.01	118.69	122.20
2	А	383	U	N3-C2-O2	-5.01	118.69	122.20
2	А	2255	С	C6-N1-C2	-5.01	118.30	120.30
2	А	2093	С	C4'-C3'-C2'	-5.01	97.59	102.60
1	R	280	GLY	CA-C-N	-5.00	106.19	117.20
2	А	2585	С	N3-C2-O2	-5.00	118.40	121.90
18	Т	64	С	O4'-C1'-N1	5.00	112.20	108.20

There are no chirality outliers.

All (38) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	А	2280	G	Sidechain
2	А	2281	G	Sidechain
2	А	2282	G	Sidechain
2	А	2511	А	Sidechain
2	А	2513	G	Sidechain
2	А	2614	U	Sidechain
2	А	2631	А	Sidechain
4	С	154	LEU	Peptide
9	Ι	22	PRO	Peptide
1	R	2	SER	Mainchain,Peptide



Mol	Chain	Res	Type	Group
1	R	279	PHE	Peptide
1	R	281	LYS	Peptide
1	R	3	PHE	Sidechain
1	R	412	SER	Mainchain,Peptide
1	R	413	SER	Peptide
1	R	414	ALA	Peptide
1	R	415	SER	Peptide
1	R	430	LYS	Mainchain
1	R	431	TYR	Sidechain,Peptide
1	R	432	LEU	Peptide
1	R	433	ARG	Sidechain
18	Т	10	G	Sidechain
18	Т	14	А	Sidechain
18	Т	21	А	Sidechain
18	Т	25	С	Sidechain
18	Т	26	G	Sidechain
18	Т	3	G	Sidechain
18	Т	45	G	Sidechain
18	Т	46	G	Sidechain
18	Т	52	G	Sidechain
18	Т	6	С	Sidechain
18	Т	67	G	Sidechain
18	Т	68	G	Sidechain
18	Т	71	С	Sidechain
18	Т	72	С	Sidechain

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## 5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

### 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
1	R	431/570~(76%)	397~(92%)	22~(5%)	12 (3%)	5	25
4	С	273/277~(99%)	261 (96%)	12 (4%)	0	100	100
5	D	205/209~(98%)	197 (96%)	8 (4%)	0	100	100
6	Е	203/207~(98%)	189 (93%)	14 (7%)	0	100	100
7	F	176/179~(98%)	163 (93%)	13 (7%)	0	100	100
8	G	173/179~(97%)	166 (96%)	7 (4%)	0	100	100
9	Ι	131/141 (93%)	126 (96%)	5 (4%)	0	100	100
10	J	140/145~(97%)	133 (95%)	7 (5%)	0	100	100
11	К	120/122~(98%)	112 (93%)	8 (7%)	0	100	100
12	L	144/146~(99%)	140 (97%)	4 (3%)	0	100	100
13	М	136/144 (94%)	133 (98%)	3 (2%)	0	100	100
14	N	117/120~(98%)	113 (97%)	4 (3%)	0	100	100
15	Ο	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
16	Q	115/119~(97%)	110 (96%)	5 (4%)	0	100	100
17	S	107/113~(95%)	94 (88%)	13 (12%)	0	100	100
19	U	98/103~(95%)	87 (89%)	11 (11%)	0	100	100
20	V	80/94~(85%)	80 (100%)	0	0	100	100
21	W	5/7~(71%)	5 (100%)	0	0	100	100
22	Х	56/62~(90%)	51 (91%)	5 (9%)	0	100	100
23	Z	56/59~(95%)	55 (98%)	1 (2%)	0	100	100
24	a	112/115~(97%)	107 (96%)	5 (4%)	0	100	100
25	b	52/59~(88%)	48 (92%)	4 (8%)	0	100	100
26	с	46/49~(94%)	46 (100%)	0	0	100	100
27	d	42/44~(96%)	42 (100%)	0	0	100	100
28	е	62/66~(94%)	59 (95%)	3 (5%)	0	100	100
29	f	34/37~(92%)	33 (97%)	1 (3%)	0	100	100
30	g	99/102~(97%)	86 (87%)	13 (13%)	0	100	100
31	h	91/95~(96%)	87 (96%)	4 (4%)	0	100	100
32	i	63/66~(96%)	59 (94%)	4 (6%)	0	100	100
All	All	3485/3749~(93%)	3292 (94%)	181 (5%)	12 (0%)	44	73

All (12) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	R	414	ALA
1	R	431	TYR
1	R	432	LEU
1	R	433	ARG
1	R	223	LEU
1	R	413	SER
1	R	429	GLY
1	R	366	ASN
1	R	416	PRO
1	R	164	LEU
1	R	176	ALA
1	R	415	SER

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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
1	R	383/505~(76%)	348~(91%)	35~(9%)	9 33
4	$\mathbf{C}$	223/225~(99%)	223~(100%)	0	100 100
5	D	168/170~(99%)	168 (100%)	0	100 100
6	Ε	169/170~(99%)	169 (100%)	0	100 100
7	F	153/154~(99%)	151 (99%)	2(1%)	69 87
8	G	148/151~(98%)	148 (100%)	0	100 100
9	Ι	103/110~(94%)	103 (100%)	0	100 100
10	J	120/123~(98%)	120 (100%)	0	100 100
11	Κ	101/101~(100%)	101 (100%)	0	100 100
12	L	110/110~(100%)	108~(98%)	2(2%)	59 82
13	М	111/116~(96%)	111 (100%)	0	100 100
14	Ν	99/100~(99%)	99 (100%)	0	100 100
15	Ο	93/93~(100%)	93 (100%)	0	100 100
16	Q	$9\overline{6}/98~(98\%)$	95~(99%)	1 (1%)	76 90
17	S	90/93~(97%)	90 (100%)	0	100 100



Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
19	U	84/87~(97%)	84 (100%)	0	100	100
20	V	64/74~(86%)	64 (100%)	0	100	100
22	Х	47/50~(94%)	46 (98%)	1 (2%)	53	79
23	Z	52/53~(98%)	52 (100%)	0	100	100
24	a	99/100~(99%)	99 (100%)	0	100	100
25	b	48/53~(91%)	48 (100%)	0	100	100
26	с	46/47~(98%)	46 (100%)	0	100	100
27	d	39/39~(100%)	38~(97%)	1 (3%)	46	74
28	е	54/56~(96%)	54 (100%)	0	100	100
29	f	34/35~(97%)	34 (100%)	0	100	100
30	g	83/84~(99%)	83 (100%)	0	100	100
31	h	84/85~(99%)	84 (100%)	0	100	100
32	i	56/57~(98%)	56 (100%)	0	100	100
All	All	2957/3139~(94%)	2915 (99%)	42 (1%)	68	86

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	3	PHE
1	R	4	ASP
1	R	26	LYS
1	R	162	TYR
1	R	163	LYS
1	R	175	GLU
1	R	179	ASP
1	R	180	ASP
1	R	220	LYS
1	R	222	THR
1	R	223	LEU
1	R	236	GLU
1	R	238	ARG
1	R	239	PHE
1	R	263	GLU
1	R	265	ARG
1	R	279	PHE
1	R	281	LYS
1	R	336	LEU



		1	1 0
$\mathbf{Mol}$	Chain	Res	Type
1	R	340	LYS
1	R	344	LYS
1	R	351	TYR
1	R	359	ILE
1	R	366	ASN
1	R	379	LYS
1	R	413	SER
1	R	417	ARG
1	R	419	ILE
1	R	420	SER
1	R	421	GLU
1	R	428	GLU
1	R	430	LYS
1	R	431	TYR
1	R	432	LEU
1	R	434	PRO
7	F	110	ARG
7	F	115	ARG
12	L	70	ASN
12	L	116	LYS
16	Q	92	ARG
22	Х	58	LYS
27	d	25	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	335	ASN
1	R	366	ASN
1	R	372	ASN
1	R	381	GLN

#### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
18	Т	75/76~(98%)	23~(30%)	6 (8%)
2	А	2916/2918~(99%)	643~(22%)	44 (1%)
3	В	111/112~(99%)	30~(27%)	2(1%)
All	All	3102/3106~(99%)	696~(22%)	52 (1%)



All (696) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A	13	A
2	А	15	G
2	А	31	С
2	А	33	U
2	А	34	U
2	А	35	G
2	А	39	С
2	А	44	А
2	А	45	G
2	А	46	С
2	А	51	G
2	А	59	G
2	А	63	G
2	А	71	A
2	А	75	G
2	А	76	С
2	А	87	U
2	А	91	А
2	А	94	А
2	А	101	G
2	А	117	А
2	А	118	А
2	А	119	U
2	А	124	А
2	А	125	А
2	А	130	А
2	А	133	А
2	А	159	U
2	A	162	A
2	A	163	U
2	А	164	U
2	A	176	A
2	А	177	G
2	A	178	A
2	А	183	A
2	A	184	G
2	A	188	C
2	A	199	A
2	A	202	A
2	А	203	U
2	A	207	A
2	А	216	A



Mol	Chain	Res	Type
2	А	219	А
2	А	225	A
2	А	226	A
2	А	227	G
2	А	230	A
2	А	231	A
2	А	233	G
2	А	236	А
2	А	245	G
2	А	251	G
2	А	252	С
2	А	253	G
2	А	258	A
2	А	267	С
2	А	268	A
2	А	269	G
2	А	270	С
2	А	272	С
2	А	275	A
2	А	282	G
2	А	289	С
2	А	290	U
2	А	291	С
2	А	295	G
2	А	298	U
2	А	299	U
2	А	300	G
2	А	301	U
2	А	302	A
2	А	310	С
2	A	312	G
2	А	313	U
2	A	314	A
2	A	315	С
2	A	321	U
2	A	322	A
2	А	324	A
2	А	325	A
2	А	331	С
2	А	337	A
2	А	345	A
2	А	346	G



Mol	Chain	Res	Type
2	А	348	U
2	А	352	G
2	А	354	А
2	А	355	A
2	А	360	С
2	А	367	G
2	А	373	А
2	А	374	А
2	А	376	А
2	А	378	С
2	А	382	G
2	А	386	U
2	А	387	С
2	А	390	A
2	А	392	С
2	А	393	U
2	А	394	U
2	А	405	U
2	А	406	G
2	А	410	G
2	А	411	G
2	А	414	С
2	А	417	G
2	А	418	А
2	А	430	С
2	А	432	С
2	А	433	G
2	А	434	U
2	А	435	G
2	А	438	А
2	A	443	G
2	A	444	U
2	А	459	A
2	A	474	U
2	A	478	U
2	A	482	С
2	A	483	С
2	A	484	C
2	А	485	U
2	A	490	A
2	A	494	A
2	А	498	U



Mol	Chain	Res	Type
2	А	502	С
2	А	503	С
2	А	504	А
2	А	514	G
2	А	528	G
2	А	538	А
2	А	548	А
2	А	550	G
2	А	551	А
2	А	552	G
2	А	554	U
2	А	555	С
2	А	556	С
2	А	558	G
2	А	562	С
2	А	564	G
2	А	572	A
2	А	576	G
2	А	577	U
2	А	578	A
2	А	592	A
2	А	593	А
2	А	594	С
2	А	595	G
2	А	607	G
2	А	617	G
2	А	619	А
2	А	631	G
2	А	647	А
2	А	648	G
2	A	649	G
2	A	650	U
2	А	651	U
2	A	660	G
2	A	663	G
2	A	666	G
2	A	667	A
2	A	673	A
2	A	674	G
2	A	680	G
2	A	683	A
2	А	684	G



Mol	Chain	Res	Type
2	А	691	U
2	А	700	U
2	А	701	G
2	А	713	G
2	А	715	А
2	А	717	А
2	А	718	С
2	А	719	С
2	А	733	U
2	А	773	G
2	А	777	С
2	А	781	А
2	А	782	A
2	А	786	A
2	А	792	G
2	А	794	U
2	А	795	G
2	А	797	A
2	А	822	G
2	А	823	G
2	А	824	G
2	А	829	A
2	А	831	U
2	А	832	G
2	А	836	А
2	А	837	U
2	А	838	С
2	А	839	G
2	А	852	G
2	А	853	С
2	А	858	U
2	А	859	С
2	А	866	A
2	А	874	U
2	А	875	U
2	А	877	G
2	А	892	U
2	А	893	A
2	А	895	G
2	А	913	A
2	А	914	С
2	А	924	U



Mol	Chain	Res	Type
2	А	925	А
2	А	927	G
2	А	928	G
2	А	931	С
2	А	935	А
2	А	937	С
2	А	942	U
2	А	943	А
2	А	944	С
2	А	948	А
2	А	951	С
2	А	952	А
2	А	954	U
2	A	957	A
2	A	959	С
2	A	961	С
2	A	962	С
2	А	964	А
2	А	973	G
2	А	977	U
2	А	978	А
2	А	981	С
2	А	987	А
2	А	988	G
2	А	990	С
2	А	991	А
2	А	992	G
2	А	999	А
2	A	1005	A
2	А	1007	G
2	А	1019	А
2	A	1020	А
2	А	1025	А
2	A	1026	А
2	A	1027	A
2	A	1028	С
2	A	1029	A
2	А	1031	С
2	A	1034	A
2	А	1037	С
2	A	1055	А
2	А	1058	U



Mol	Chain	Res	Type
2	А	1059	А
2	А	1068	G
2	А	1072	А
2	А	1079	U
2	А	1091	U
2	А	1092	А
2	А	1093	G
2	А	1102	G
2	А	1104	U
2	А	1105	G
2	А	1107	U
2	A	1108	G
2	A	1110	С
2	А	1111	U
2	А	1112	U
2	А	1113	А
2	А	1115	А
2	А	1116	А
2	А	1117	G
2	А	1123	А
2	А	1124	С
2	А	1127	U
2	А	1128	U
2	А	1129	U
2	А	1131	А
2	А	1135	G
2	А	1139	G
2	А	1140	U
2	А	1141	А
2	А	1142	А
2	A	1143	U
2	A	1144	А
2	A	1152	G
2	A	1157	A
2	A	1158	G
2	A	1159	U
2	A	1176	U
2	A	1178	U
2	A	1179	A
2	A	1181	С
2	A	1182	G
2	А	1185	G



Mol	Chain	Res	Type
2	А	1187	U
2	А	1188	A
2	А	1194	А
2	А	1201	А
2	А	1202	А
2	А	1209	G
2	А	1217	U
2	А	1218	U
2	А	1219	С
2	А	1220	G
2	А	1246	G
2	А	1247	G
2	А	1251	U
2	А	1252	G
2	А	1260	A
2	А	1276	G
2	А	1278	G
2	А	1289	U
2	А	1293	А
2	А	1295	U
2	А	1296	G
2	А	1311	G
2	А	1312	А
2	А	1313	А
2	А	1314	А
2	А	1315	G
2	А	1327	U
2	А	1339	А
2	А	1340	А
2	А	1345	U
2	A	1346	A
2	A	1352	U
2	А	1363	G
2	A	1364	С
2	A	1376	G
2	A	1381	A
2	А	1382	G
2	А	1384	С
2	A	1388	A
2	A	1404	A
2	А	1417	A
2	А	1418	U



Mol	Chain	Res	Type
2	А	1423	А
2	А	1424	А
2	А	1425	С
2	А	1431	G
2	А	1433	U
2	А	1435	U
2	А	1436	U
2	А	1439	U
2	А	1441	U
2	А	1442	А
2	А	1450	С
2	А	1456	А
2	А	1460	G
2	А	1464	А
2	А	1472	G
2	А	1473	А
2	А	1474	С
2	А	1490	А
2	А	1497	G
2	А	1498	U
2	А	1499	А
2	А	1507	U
2	А	1513	U
2	А	1519	С
2	А	1520	А
2	А	1524	А
2	А	1528	U
2	А	1536	А
2	А	1539	С
2	А	1553	A
2	А	1555	A
2	A	1561	G
2	A	1563	G
2	A	1564	С
2	А	1569	A
2	A	1571	G
2	А	1572	G
2	A	1573	С
2	A	1581	A
2	A	1582	U
2	A	1584	U
2	А	1586	G



Mol	Chain	Res	Type
2	А	1596	U
2	А	1607	С
2	А	1608	А
2	А	1614	А
2	А	1617	А
2	А	1626	U
2	А	1631	А
2	А	1632	G
2	А	1634	U
2	А	1652	С
2	А	1653	А
2	А	1655	А
2	А	1657	С
2	А	1658	G
2	А	1660	С
2	А	1667	А
2	А	1674	G
2	А	1679	А
2	А	1691	А
2	А	1692	U
2	А	1693	С
2	А	1696	G
2	А	1697	А
2	А	1705	С
2	А	1709	А
2	А	1712	G
2	А	1719	G
2	А	1727	А
2	А	1744	G
2	А	1745	А
2	A	1752	G
2	A	1756	U
2	A	1757	G
2	A	1758	U
2	A	1770	С
2	A	1774	A
2	A	1777	G
2	A	1778	A
2	A	1779	G
2	A	1780	С
2	A	1781	С
2	А	1782	G



$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Mol	Chain	Res	Type
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	А	1785	G
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	А	1788	А
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	А	1791	А
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	А	1792	G
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	А	1793	G
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	А	1802	А
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	А	1805	G
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	А	1809	А
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	А	1811	С
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	А	1829	С
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	А	1830	G
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	А	1845	А
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	А	1858	А
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	2	А	1877	А
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	А	1881	U
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	2	А	1895	А
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	А	1898	G
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	А	1901	А
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	А	1902	G
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	А	1912	G
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	2	А	1913	А
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	2	А	1918	А
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	А	1935	G
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	2	А	1941	А
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	А	1949	С
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	А	1958	G
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	А	1959	G
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	А	1966	А
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	А	1968	U
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	А	1972	U
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	А	1984	U
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	А	1990	С
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	А	1993	G
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	А	1996	С
2 A 2000 A	2	А	1999	A
$2 \qquad \Lambda \qquad 2001 \qquad C$	2	А	2000	A
2 A 2001 G	2	А	2001	G
2 A 2011 U	2	А	2011	U
2 A 2020 U	2	А	2020	U
2 A 2021 G	2	А	2021	G
2 A 2022 U	2	А	2022	U
2 A 2024 U	2	А	2024	U



Mol	Chain	Res	Type
2	А	2026	А
2	А	2050	G
2	А	2052	А
2	А	2060	А
2	А	2061	G
2	А	2062	А
2	А	2068	G
2	А	2072	С
2	А	2084	С
2	А	2085	G
2	А	2088	А
2	А	2089	А
2	А	2090	G
2	А	2091	А
2	А	2098	G
2	А	2110	С
2	А	2111	А
2	А	2121	U
2	А	2123	А
2	А	2140	U
2	А	2142	С
2	А	2143	А
2	А	2145	G
2	А	2147	U
2	А	2149	G
2	А	2155	А
2	А	2156	G
2	А	2157	С
2	А	2161	G
2	А	2162	G
2	А	2165	А
2	А	2175	С
2	А	2176	А
2	А	2177	G
2	A	2187	A
2	A	2195	G
2	А	2197	G
2	A	2200	A
2	А	2232	G
2	A	2233	С
2	A	2235	G
2	А	2240	U



Mol	Chain	Res	Type
2	А	2241	А
2	А	2243	С
2	А	2254	А
2	А	2255	С
2	А	2267	G
2	А	2268	G
2	А	2308	G
2	А	2311	G
2	А	2312	С
2	А	2315	А
2	А	2317	А
2	А	2333	G
2	А	2334	U
2	А	2335	U
2	А	2336	G
2	А	2337	G
2	А	2338	А
2	А	2345	U
2	А	2346	С
2	А	2348	С
2	А	2349	А
2	А	2350	G
2	А	2351	А
2	А	2352	G
2	А	2356	А
2	А	2357	А
2	А	2363	С
2	А	2364	А
2	А	2374	G
2	А	2377	U
2	A	2379	С
2	А	2390	А
2	А	2408	G
2	А	2411	G
2	А	2412	G
2	А	2414	С
2	А	2420	G
2	А	2431	U
2	А	2435	С
2	А	2436	А
2	А	2454	А
2	А	2455	А



Mol	Chain	Res	Type
2	А	2457	G
2	А	2458	G
2	А	2459	А
2	А	2464	А
2	А	2468	А
2	А	2469	С
2	А	2470	С
2	А	2476	G
2	А	2477	А
2	А	2486	U
2	А	2488	А
2	А	2502	U
2	А	2505	А
2	А	2507	А
2	А	2519	G
2	А	2523	G
2	А	2527	С
2	А	2528	С
2	А	2531	G
2	А	2532	А
2	А	2534	G
2	А	2535	U
2	А	2542	А
2	А	2549	С
2	А	2558	G
2	А	2564	G
2	А	2572	G
2	А	2577	G
2	А	2583	U
2	А	2593	А
2	А	2594	А
2	A	2595	A
2	A	2596	G
2	A	2598	G
2	A	2601	A
2	A	2607	G
2	A	2611	G
2	A	2619	A
2	A	2631	A
2	A	2632	G
2	A	2638	U
2	А	2639	C



Mol	Chain	Res	Type
2	А	2642	U
2	А	2644	U
2	А	2648	U
2	А	2658	А
2	А	2659	G
2	А	2675	С
2	А	2676	U
2	А	2683	А
2	А	2702	G
2	А	2710	С
2	А	2711	G
2	А	2714	G
2	А	2717	G
2	А	2718	U
2	А	2720	С
2	А	2743	G
2	А	2754	А
2	А	2755	U
2	А	2762	A
2	А	2764	G
2	А	2768	U
2	А	2773	G
2	А	2777	A
2	А	2779	A
2	А	2785	U
2	А	2786	A
2	А	2794	A
2	А	2795	G
2	А	2797	С
2	А	2799	С
2	А	2804	A
2	А	2807	A
2	А	2808	U
2	А	2813	U
2	А	2818	С
2	А	2819	A
2	А	2820	U
2	А	2825	С
2	А	2826	A
2	А	2828	G
2	А	2830	A
2	А	2845	A



Mol	Chain	Res	Type
2	А	2855	G
2	А	2858	U
2	А	2859	G
2	А	2860	А
2	А	2861	U
2	А	2874	G
2	А	2897	G
2	А	2898	А
2	А	2899	С
2	А	2905	С
2	А	2908	А
2	А	2918	G
2	А	2921	U
3	В	10	G
3	В	11	А
3	В	12	U
3	В	13	А
3	В	14	G
3	В	19	G
3	В	20	А
3	В	23	U
3	В	28	С
3	В	33	U
3	В	38	U
3	В	39	А
3	В	40	С
3	В	41	С
3	В	42	G
3	В	48	G
3	В	49	G
3	В	51	A
3	В	54	U
3	В	55	A
3	В	59	U
3	В	60	C
3	В	64	A
3	В	85	U
3	В	86	U
3	В	87	U
3	В	88	С
3	В	97	A
3	В	107	G



Mol	Chain	$\mathbf{Res}$	Type
3	В	110	G
18	Т	16	С
18	Т	17	U
18	Т	18	G
18	Т	19	G
18	Т	20	G
18	Т	34	U
18	Т	36	С
18	Т	38	С
18	Т	41	А
18	Т	44	А
18	Т	45	G
18	Т	46	G
18	Т	48	С
18	Т	53	G
18	Т	55	U
18	Т	57	G
18	Т	65	U
18	Т	66	А
18	Т	67	G
18	Т	70	U
18	Т	71	С
18	Т	73	А
18	Т	74	С

All (52) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	А	12	А
2	А	43	G
2	А	58	G
2	А	90	А
2	А	175	G
2	А	183	А
2	А	229	А
2	А	288	С
2	А	377	G
2	А	405	U
2	А	437	А
2	А	537	А
2	А	549	А
2	А	649	G



Mol	Chain	Res	Type
2	А	662	U
2	А	683	А
2	А	717	А
2	А	785	С
2	А	837	U
2	А	936	С
2	А	1111	U
2	А	1245	G
2	А	1250	G
2	А	1351	U
2	А	1362	G
2	А	1438	С
2	А	1595	U
2	А	1630	G
2	А	1652	С
2	А	1755	С
2	А	1779	G
2	А	1784	A
2	А	1948	A
2	А	2267	G
2	А	2334	U
2	А	2351	A
2	А	2454	A
2	А	2468	A
2	А	2710	С
2	А	2716	U
2	А	2784	С
2	А	2785	U
2	А	2796	С
2	А	2812	A
3	В	47	С
3	В	59	U
18	Т	7	U
18	Т	9	A
18	Т	65	U
18	Т	70	U
18	Т	72	С
18	Т	74	С

## 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	А	1
1	R	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1941:A	O3'	1947:A	Р	13.89
1	R	429:GLY	С	430:LYS	Ν	1.65



# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11864. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

## 6.1 Orthogonal projections (i)

#### 6.1.1 Primary map



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

### 6.2 Central slices (i)

#### 6.2.1 Primary map



X Index: 192



Y Index: 192



Z Index: 192

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: 207

Y Index: 211

Z Index: 183

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

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

#### 6.4.1 Primary map



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



### 6.5 Orthogonal surface views (i)

#### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0085. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.6 Mask visualisation (i)

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



# 7 Map analysis (i)

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

## 7.1 Map-value distribution (i)



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



### 7.2 Volume estimate (i)



The volume at the recommended contour level is  $1417 \text{ nm}^3$ ; this corresponds to an approximate mass of 1280 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 0.323  ${\rm \AA}^{-1}$ 



# 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-11864 and PDB model 7AQD. 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 0.0085 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 (0.0085).



### 9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

### 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0085) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9350	0.4100
А	0.9770	0.4440
В	0.9910	0.3430
С	0.9460	0.4690
D	0.9260	0.4670
Е	0.9180	0.4290
F	0.7530	0.1490
G	0.8670	0.2700
Ι	0.2700	0.0450
J	0.9320	0.4600
K	0.9240	0.4510
L	0.9140	0.4340
М	0.9080	0.4340
Ν	0.9190	0.4590
0	0.8580	0.2800
Q	0.9330	0.4580
R	0.5430	0.0770
S	0.9430	0.4780
Т	0.9010	0.1850
U	0.8960	0.3700
V	0.8870	0.4450
W	0.9430	0.3940
Х	0.9190	0.4060
Z	0.9120	0.4400
a	0.8900	0.4200
b	0.9470	0.4660
с	0.9280	0.4190
d	0.9650	0.5350
е	0.9500	0.4980
f	0.9110	0.4320
g	0.8920	0.4090
h	0.8910	0.4040
i	0.8770	0.3100

