

# wwPDB EM Validation Summary Report (i)

Oct 28, 2024 - 09:59 am GMT

PDB ID	:	5GAH
EMDB ID	:	EMD-8004
Title	:	RNC in complex with SRP with detached NG domain
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Deposited on	:	2015-11-26
Resolution	:	3.80 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:

EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
$\operatorname{MapQ}$	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

# 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 3.80 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM\ structures}\ (\#{f Entries})$		
Clashscore	210492	15764		
Ramachandran outliers	207382	16835		
Sidechain outliers	206894	16415		
RNA backbone	6643	2191		

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 cha	in	
1	1	113	17% 18%		62%	
2	2	3	33%	33%	33%	
3	А	2903	<b>•</b> 54%		37%	8% ••
4	В	120		74%	229	<i>1</i> 6 •
5	С	273	•	70%	26%	•••
6	D	209		78%		20% •
7	Е	201		77%	2	0% •

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Chain Length Quality of chain Mol i. 8 F 17935% 60% • • i ••• 9  $\mathbf{G}$ 17769% 29% 24% 10 Η 149• 66% 32% 15% Ι 11 16550% 25% 24% • 35% J 1214254% 37% • 6% 13Κ 14273% 23% • L 1231468% 30% • i . М 1514474% 24% Ν 16136. 72% 26% Ο 1712770% 25% • • ÷ Р 1811765% 32% • ••• Q 1911574% 24% i. 20R 118. . 74% 21% i  $\mathbf{S}$ 2110370% 28% • ÷ 22Т • 11078% 20% ÷ 23U 100• 5% 71% 23% V • • 2410468% 29% W 94 . 2574% 24% Х 2685 59% 28% 11% • i. ••• 27Υ 7862% 36% ÷ Ζ 2863 67% 27% 5%• . . 2959 $\mathbf{a}$ 95% • 30 b 5777% 21% 31 $\mathbf{c}$ 5584% 7% 9% 32 d 46 87% 13%

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Mol	Chain	Length	Quality of chain	
33	е	65	92%	6% •
34	f	38	92%	8%
35	i	453	9% 26% • 72%	
36	k	18	89%	11%



# 2 Entry composition (i)

There are 38 unique types of molecules in this entry. The entry contains 94027 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 SRP 4.5S RNA.

Mol	Chain	Residues		$\mathbf{A}$	toms	AltConf	Trace		
1	1	43	Total 926	C 413	N 174	0 296	Р 43	0	0

• Molecule 2 is a RNA chain called tRNA CCAend.

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

• Molecule 3 is a RNA chain called 23S rRNA.

Mol	Chain	Residues		-	AltConf	Trace			
3	А	2883	Total 61902	C 27613	N 11397	O 20009	Р 2883	0	0

• Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues		At	AltConf	Trace			
4	В	120	Total 2569	C 1144	N 468	O 837	Р 120	0	0

• Molecule 5 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	С	271	Total 2082	C 1288	N 423	0 364	${ m S} 7$	0	0

• Molecule 6 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	209	Total 1565	C 979	N 288	0 294	${S \atop 4}$	0	0



• Molecule 7 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues		At	oms	AltConf	Trace		
7	Е	201	Total 1552	С 974	N 283	O 290	${ m S}{ m 5}$	0	0

• Molecule 8 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues		At	AltConf	Trace			
8	F	177	Total 1410	C 899	N 249	O 256	S 6	0	0

• Molecule 9 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues		At	oms			AltConf	Trace
9	G	176	Total 1323	C 832	N 243	0 246	$\frac{S}{2}$	0	0

• Molecule 10 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues		At	oms			AltConf	Trace
10	Н	149	Total	С	Ν	0	$\mathbf{S}$	0	0
10	11	110	1110	699	197	213	1	0	0

• Molecule 11 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues		At	oms		Atoms					
11	Ι	125	Total 946	C 599	N 169	0 175	${ m S} { m 3}$	0	0			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ι	85	VAL	SER	conflict	UNP P0A7J3
Ι	86	THR	MET	conflict	UNP P0A7J3

• Molecule 12 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues		At	AltConf	Trace			
12	J	134	Total 979	C 619	N 169	0 185	S 6	0	0

• Molecule 13 is a protein called 50S ribosomal protein L13.



Mol	Chain	Residues		At	oms			AltConf	Trace
13	K	142	Total 1129	C 714	N 212	0 199	$\frac{S}{4}$	0	0

• Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues		At	oms			AltConf	Trace
14	L	123	Total 946	C 593	N 181	O 166	S 6	0	0

• Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues		At	AltConf	Trace			
15	М	144	Total 1053	C 654	N 207	O 190	${S \over 2}$	0	0

• Molecule 16 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues		At	AltConf	Trace			
16	Ν	136	Total 1074	C 686	N 205	0 177	S 6	0	0

• Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues		At	AltConf	Trace			
17	О	125	Total 993	C 613	N 202	0 173	${ m S}{ m 5}$	0	0

• Molecule 18 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues		At	AltConf	Trace			
18	Р	117	Total 900	C 557	N 179	0 163	S 1	0	0

• Molecule 19 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues		At	oms			AltConf	Trace
19	Q	114	Total 917	С 574	N 179	0 163	S 1	0	0

• Molecule 20 is a protein called 50S ribosomal protein L20.



Mol	Chain	Residues		Ato	ms		AltConf	Trace
20	R	117	Total 947	C 604	N 192	O 151	0	0

• Molecule 21 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues		At	oms		AltConf	Trace	
21	S	103	Total 816	C 516	N 153	0 145	${S \over 2}$	0	0

• Molecule 22 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues		At	oms		AltConf	Trace	
22	Т	110	Total 857	C 532	N 166	0 156	${ m S} { m 3}$	0	0

• Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues		At	oms		AltConf	Trace	
23	U	95	Total 756	C 479	N 141	0 135	S 1	0	0

• Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
24	V	102	Total 779	C 492	N 146	0 141	0	0

• Molecule 25 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues		At	$\mathbf{oms}$		AltConf	Trace	
25	W	94	Total 753	C 479	N 137	0 134	${ m S} { m 3}$	0	0

• Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues		At	oms		AltConf	Trace	
26	Х	76	Total 580	C 359	N 117	0 103	S 1	0	0

• Molecule 27 is a protein called 50S ribosomal protein L28.



Mol	Chain	Residues		At	oms			AltConf	Trace
27	Y	77	Total 625	C 388	N 129	O 106	${ m S} { m 2}$	0	0

• Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
28	Z	62	Total	С	N	0	S	0	0
			501	308	98	94	T		

• Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
29	a	58	Total 449	C 281	N 87	O 79	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
30	h	56	Total	С	Ν	Ο	$\mathbf{S}$	0	0
50	U	50	444	269	94	80	1	0	0

• Molecule 31 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues		Aton	ıs	AltConf	Trace	
31	с	51	Total 414	C 266	N 76	O 72	0	0

• Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
32	d	46	Total 377	C 228	N 90	O 57	${ m S} { m 2}$	0	0

• Molecule 33 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues		Ate	oms	AltConf	Trace		
33	е	64	Total 504	C 323	N 105	0 74	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 34 is a protein called 50S ribosomal protein L36.



Mol	Chain	Residues		Atc	$\mathbf{ms}$	AltConf	Trace		
34	f	38	Total	C	N CT	0	S	0	0
			302	185	05	48	4		

• Molecule 35 is a protein called Signal recognition particle protein Ffh.

Mol	Chain	Residues		$\mathbf{A}$	toms	AltConf	Trace		
35	i	126	Total 916	C 575	N 169	0 161	S 11	0	0

• Molecule 36 is a protein called 1A9L SS.

Mol	Chain	Residues		Ate	$\mathbf{oms}$	AltConf	Trace		
36	k	18	Total 137	C 94	N 20	O 22	S 1	0	0

• Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
37	2	1	Total Mg 1 1	0
37	А	412	Total         Mg           412         412	0
37	В	11	Total Mg 11 11	0
37	С	2	Total Mg 2 2	0
37	D	1	Total Mg 1 1	0
37	Ε	1	Total Mg 1 1	0
37	Р	1	Total Mg 1 1	0
37	R	1	Total Mg 1 1	0
37	b	1	Total Mg 1 1	0

• Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
38	f	1	Total Zn 1 1	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.



 $\bullet$  Molecule 1: SRP 4.5S RNA



A504	A505	CE09	C510	0511 G512	A513	A514 A515	C516	C517	4010 U519	G520	U521	A526	C527	A528 A529	G530	C531	Ab 32 G5 33		G543 CEAA	U545	n ·	A G548	G549	C550	U552	II558		G561 U562	A563	C564 C565	U566	U567 U568	U569 0570	u571	A572	05/3 A574	A575	G577	C581	G585
A586	II591	A592	<b>U593</b>	0594 0595		C601 A602	A603	G604	000	A 608	A609	C611 C611	G612	A613 A614	U615	A616	G620	A621	G622	A627	G628	G630	A631	A632 A633	C634	4637	G638	U639 C640	U641	0642	C645	0646 G647	G648	C650	0.000	0653 A654	A655	U657		A668 G669
A670	C671 C672	C673	G674	A677	C678	C679 C680	G681	A C OF			A706 6707		G711	G712 G713	U714	1	C/1/ A718	C7 19	U720 A721	A722		67.29 A7.30		G733	G738	11741	A742	A743	U746	U747	A753	U/ 54 U7 55	A756	G758	G759	G763	A764 C765		U773	G774 G775
G776	6777 6778	0779	G780	A781 A782	A783	G784 G785		A788	01790	C791	A792 A703	A794	C795	C796 G797	G798	6299	<b>A</b> 800 <b>G</b> 801		A804 CR05	C806	U807	6809	U810	U811	U813	C815	C816	<u>A819</u>		G822 C823	U824	4825 U826	U827	00200 A829	<mark>6830</mark>	6831 U832	A833	0035 C835	U839	C840
A845	U846 11847	C848	A849	U850	G857	G858 G859	<b>U860</b>	A861 7860	4862 A863	G864	C865	<mark>G869</mark>	<mark>0870</mark>	U871 11872		C876	A877 A878	<mark>G879</mark>	G880	G882	<del>ت</del> :	ס ט	Ä	Þ	00	0 5	Ä	С <mark>1894</mark>	U895	A896	C898	A899	000	0602 0608	A909	A910 A911		G914 C915	G916 A917	<mark>6930</mark>
U931	0932 4933	00004	C946	A947 C948	G949	1023 1023		C957	A959	A960	C961	C968	6969	0970 0971	A972	A973	G974 A975	6976	AQ8 1	C982	A983	A364	C987		C991	C992	C994	C995 A996	6997	C998 U999	A1000	A1001 G1002	27 27 20	C1006	C1007	A1008 A1009	A1010	U1012	CTOTO	A1021 G1022
U1023	61024 61025	G1026	A1027	A1028	U1033	<mark>G1038</mark>	A1039	A1040	C1044	C1045	A1046	A1048		G1056 A1057		U1060	01061 G1062	G1063	C1064	U1066	A1067	G1068	A1069 A1070	G1071	<mark>C1072</mark> A1073	G1074	C1075	A1077	01078 C1079	111082	U1083	A1084	A1086	G1087 A1088	A1089	A1090	<mark>G1093</mark>	U1094 A1095	A1096 U1097	A1098 G1099
C1100	01101 C1102	A1103	C1104	01105 01106		G1110 A1111	G1112	<b>11</b> 1	G1115 G1116		G1125 A1126	A1127	G1128	A1129 III 130	G1131	U1 132	A1133 A1134	C1135	<mark>G1136</mark>	G1139	C1140	01141 A1142	A1143	140	C1150	G1154	A1 155	G1168	A1169	C1170 C1171	C1172	U11/3	A	0 G1177	C1178	011/9 01180	U1181 C1182	70110	u1188	U1198
<mark>U1199</mark>	A1 205	G1206		G1210 C1211	G1212	G1 01 8		A1230		<mark>G1236</mark>	A1237 G1738		C1243	A1 247	G1248	U1249	G1250 C1251	G1252	A1253	01255	G1256	UL257 111258	G1259	A1260	A1262	G1 266	U1267	A1268 A1269	C1270	G1271 A1272	100	412/9	A1287	G1 289	<mark>C1290</mark>	U1294	r1 300	A1301	61303 G1303	A1308
_	01313 01314		A1321	G1324		A1327 A1328	U1329	1000	0 1002	G1337	G1338 C1230	U1340	G1341	A1342 C1343	U1344	C1345	G1340	c1351	A126/	G1355	000	C1362 C1363	G1364	A1365 A1366	A1367	01374 01374		U1379	A1383	c1386	A1387	61388	U1394	A1390 U1396	U1397	C1398 C1399	01400 01401	01402	A1403 C1404	U1405 U1406
_	31410	C1414	J1415	31416	1418	41419 41420	31421	31422 1422	1423 31424	31425	31426 1427	C1428		31432 M1433	41434	31435	c1437	11438	<b>A1439</b>	J1442	<mark>J1443</mark>	1446	01447	31448 1446	1450	01451 01450	A1453	1463 11463	31464	11465 J1466	J1467	01468 A1469	A1470	31473	<mark>J1474</mark>	31482	31483 11 / 8 /	11485	<b>C1489</b>	41490 31491
1492	1493 1494	1495	1496	1497 1498	1499	1500 1501	1502		1507 (	1508	1509	1511 (		1515 1516	1517		1524 1525	1526	1527 1528	1529 1529	1530	1531 1532	1533	1534 1536	1536	1537	1542	1543 1544	1545	1546	1554	1560		1564 (	1565 1565		1569 ( 1570	1571	7 /01	1576 1577
1578 C	1281 1281	1582 A	1583 A	1584 1585		1590 1591	1592 A	1 1 1	1598 C	V	1603 1604	1605 G	1606	1607	1609	1610	1614 A	1615 C	1616 1617		1627 200		1631 G	1 V		1637 1638	1 <u>6</u> 39	16 1642	1643 A	1645 1645	1646 1545	1648 G	1649	1652	1653	1655	L ED	1660 1660	1664	1 <mark>667 C</mark>
D	672 873	574 C1	A	577 0 578 C		581 A	2389 289			200	706 A	707	708 C	709 C	711 A	A		721 C:	722 A.	725	U U U	730	731	732	135 735	736 A.	738	743 61	744 G:	751 751	752 C.	756 U1	757 G.	759 A1	760 G	762 A	763 764		770 A:	773
	5 A1(	016		2 A16	5	616	9 A16			4 A17	<u>د د</u>	2 617	8 C11	017 017	1 A17	2	2 CT	8 G17	9 A1	1 U17			8 G17	9 C11	1 A17	2 01	5 617	6 7 G17	8 A17	017 U17	7 C11	6 17 617	A11		8 C11		611 7		9 617	9 A17
C1774	U177E	A1780	U1781	U1782	A1785	A1786	A1789	C1790	TRITY	A1794	C1795	G1797	U1798	G1799 C1800	A1801	A1802	G1807	A1808	A1809	G1811		01817 01817	U1818	A1815	A1821	C1822	U1825	G1826 U1827	G1828	A1828	C1837	C1838 G1839	01010	A1847	A1848	G1850 G1850	A 1052		01859 01859	G1869





• Molecule 4: 5S rRNA



 $\bullet$  Molecule 5: 50S ribosomal protein L2





 $\bullet$  Molecule 6: 50S ribosomal protein L3



#### P152 K157 K157 K160 E168 E168 A182 R184 A196 L201 L201 L201 L201 K208 K208

• Molecule 7: 50S ribosomal protein L4



#### Π11 Π12 Π1





• Molecule 14: 50S ribosomal protein L14



 $\bullet$  Molecule 15: 50S ribosomal protein L15



• Molecule 16: 50S ribosomal protein L16



• Molecule 17: 50S ribosomal protein L17



• Molecule 18: 50S ribosomal protein L18









Chain c:	84%	9% 7%
MET ALA LYS C4 C4 K10 K10 T22	154 IS4 ITS	
• Molecule 32:	50S ribosomal protein L34	
Chain d:	87%	13%
M1 R12 R24 K25 R34 R34		
• Molecule 33:	50S ribosomal protein L35	
Chain e:	92%	6% •
MET P2 R8 H31 H31 H31 S51 S51		
• Molecule 34:	50S ribosomal protein L36	
Chain f:	92%	8%
M1 K2 R12 Q37 Q37 G38		
• Molecule 35:	Signal recognition particle protein Ffh	
Chain i:	26% · 72%	
MET PHE ASP ASN LEU THR ASP ASP LEU SER SER ARG	THR THR ARG ARG ARG ARG ARG ARG ARG ARG ARG AR	VAL LEU LEU PRO PRO PRO PRO OLU VAL CYS GLU CYS GLU CYS CLU VAL VAL
GLY HIS GLU GLU VAL ASN LYS SER LEU THR PRO GLY	CLN CLN PHE VAL LYS LLYS LLYS VAL ARG CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	VAL MET MET MET MET ALA ALA ALA ALA ALA ALA ALA ALA CIN CIN CIN CIN CIN CIN CIN CIN CIN CIN
CLY LYS PHE LEU ARG GLU CLYS HIS LYS LYS LYS	VAL LEU VAL VAL SER SER ASP ASP ASP ARG ALA ALA ALA ALA ALA ALA ALA ALA ALA CLU GLU CLU CLU CLU CLU SER SER SER SER SER SER SER SER SER SER	ASP VAL GLN GLN CJLN PPO CJLN VAL ASP ALA ALA ALA ALA ALA ALA ALA ALA ALA AL
LEU LYS LYS PHE ASP ASP VAL LEU VAL LEU VAL ASP ASP	ALA ALA GLY ARG ALY ARC ALU ASP ALU ACL ASP ALU ACL ACL ALA ALA ALA ALA ALA ALA ALA ALA	ALA THET THET THE THE GLY GLY ALA ALA ALA ALA ALA ALA ALA ALA ALA A
PRO LEU THR GLY VAL VAL LEU LEU LAS VAL ASP	GLY ALSP ALSP ALSP ALS ALS ALA ALA ALA ALA LEU LEU CLY GLY CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	CLU PHE PHE ARC ARC ARC ARC ARC ARC ARC ARC ARC ARC
LEU SER LEU LEU ILE GLU GLU GLU SER LYS VAL	ASP ARA ALA ALA ALA ALA ALA ALA CLU SER ALA CLU SER ALA CLU SER ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	Kind Made Made Made Made Made Made Made Mad





• Molecule 36: 1A9L SS





# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46409	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 $(e^-/\text{\AA}^2)$	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.390	Depositor
Minimum map value	-0.215	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	398.88, 398.88, 398.88	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.385, 1.385, 1.385	Depositor



# 5 Model quality (i)

# 5.1 Standard geometry (i)

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

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

Mal	Chain	B	ond lengths	Bond angles							
1VIOI	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5						
1	1	0.79	0/1037	1.29	7/1616~(0.4%)						
2	2	0.57	0/68	1.25	1/103~(1.0%)						
3	А	0.68	14/69329~(0.0%)	1.17	187/108152~(0.2%)						
4	В	0.51	0/2872	1.04	1/4478~(0.0%)						
5	С	0.47	0/2121	0.65	0/2852						
6	D	0.47	0/1586	0.63	0/2134						
7	Ε	0.44	0/1571	0.61	1/2113~(0.0%)						
8	F	0.39	0/1434	0.56	0/1926						
9	G	0.39	0/1343	0.58	0/1816						
10	Н	0.42	0/1121	0.57	0/1515						
11	Ι	0.48	0/958	0.62	1/1292~(0.1%)						
12	J	0.58	0/993	0.69	1/1341~(0.1%)						
13	Κ	0.46	0/1152	0.57	0/1551						
14	L	0.45	0/955	0.63	0/1279						
15	М	0.47	0/1062	0.64	0/1413						
16	Ν	0.48	0/1093	0.59	0/1460						
17	0	0.47	0/1006	0.67	0/1345						
18	Р	0.41	0/910	0.56	0/1219						
19	Q	0.48	0/929	0.60	0/1242						
20	R	0.56	0/960	0.59	0/1278						
21	S	0.46	0/829	0.62	0/1107						
22	Т	0.52	0/864	0.71	0/1156						
23	U	0.45	0/763	0.61	0/1021						
24	V	0.38	0/787	0.54	0/1051						
25	W	0.40	0/766	0.57	0/1025						
26	Х	0.50	0/587	0.60	0/776						
27	Y	0.48	0/635	0.61	0/848						
28	Z	0.41	$0/\overline{502}$	0.54	$0/\overline{667}$						
29	a	0.38	0/453	0.56	0/605						
30	b	0.43	0/450	0.62	0/599						
31	с	0.44	0/421	0.61	0/561						
32	d	0.51	0/380	0.66	0/498						



Mal	Chain	B	ond lengths	Bond angles		
INIOI	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
33	е	0.47	0/513	0.62	0/676	
34	f	0.49	0/303	0.58	0/397	
35	i	0.44	0/672	0.56	0/883	
36	k	0.62	0/137	0.85	0/186	
All	All	0.63	14/101562~(0.0%)	1.05	199/152181~(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
5	С	0	1
9	G	0	1
12	J	0	1
All	All	0	3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	А	2542	А	N9-C4	-6.90	1.33	1.37
3	А	1254	А	N9-C4	-6.39	1.34	1.37
3	А	1321	А	N9-C4	6.27	1.41	1.37
3	А	1490	А	N9-C4	6.00	1.41	1.37
3	А	2114	А	N9-C4	5.98	1.41	1.37

The worst 5 of 199 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	А	2423	U	C6-N1-C2	-12.25	113.65	121.00
3	А	1838	С	C6-N1-C2	9.39	124.06	120.30
3	А	2422	С	O4'-C1'-N1	9.31	115.65	108.20
3	А	2423	U	C5-C6-N1	8.80	127.10	122.70
3	А	1584	U	C2-N1-C1'	8.52	127.92	117.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	С	232	HIS	Peptide
9	G	47	ASP	Peptide
	0		1	1

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Mol	Chain	$\operatorname{Res}$	Type	Group
12	J	19	ASN	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	1	926	0	467	10	0
2	2	62	0	34	1	0
3	А	61902	0	31133	683	0
4	В	2569	0	1301	19	0
5	С	2082	0	2154	51	0
6	D	1565	0	1616	32	0
7	Ε	1552	0	1619	27	0
8	F	1410	0	1444	42	0
9	G	1323	0	1371	35	0
10	Н	1110	0	1148	23	0
11	Ι	946	0	978	31	0
12	J	979	0	1028	39	0
13	Κ	1129	0	1162	24	0
14	L	946	0	1023	21	0
15	М	1053	0	1129	26	0
16	Ν	1074	0	1157	23	0
17	0	993	0	1034	25	0
18	Р	900	0	935	23	0
19	Q	917	0	962	19	0
20	R	947	0	1019	24	0
21	S	816	0	839	20	0
22	Т	857	0	922	14	0
23	U	756	0	817	14	0
24	V	779	0	831	18	0
25	W	753	0	780	14	0
26	Х	580	0	594	16	0
27	Y	625	0	652	17	0
28	Ζ	501	0	531	13	0
29	a	449	0	488	0	0
30	b	444	0	458	0	0
31	с	414	0	442	0	0
32	d	377	0	418	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	е	504	0	572	0	0
34	f	302	0	340	0	0
35	i	916	0	944	0	0
36	k	137	0	168	0	0
37	2	1	0	0	0	0
37	А	412	0	0	0	0
37	В	11	0	0	0	0
37	С	2	0	0	0	0
37	D	1	0	0	0	0
37	Е	1	0	0	0	0
37	Р	1	0	0	0	0
37	R	1	0	0	0	0
37	b	1	0	0	0	0
38	f	1	0	0	0	0
All	All	94027	0	62510	1167	0

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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 8.

The worst 5 of 1167 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:A:1818:U:OP2	5:C:156:ARG:NH1	2.00	0.95
3:A:1168:G:H1	3:A:1181:U:H3	1.20	0.90
3:A:276:U:O2	3:A:278:A:N6	2.08	0.87
3:A:1827:U:OP2	5:C:221:ARG:NH1	2.08	0.86
10:H:3:VAL:HG12	10:H:38:PRO:HA	1.57	0.86

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	ntiles
5	С	269/273~(98%)	261 (97%)	8(3%)	0	100	100
6	D	207/209~(99%)	201 (97%)	6(3%)	0	100	100
7	Ε	199/201~(99%)	190 (96%)	9 (4%)	0	100	100
8	F	175/179~(98%)	166 (95%)	9(5%)	0	100	100
9	G	174/177~(98%)	171 (98%)	3 (2%)	0	100	100
10	Н	147/149~(99%)	138 (94%)	8 (5%)	1 (1%)	19	52
11	Ι	123/165~(74%)	113 (92%)	9 (7%)	1 (1%)	16	49
12	J	132/142~(93%)	126 (96%)	6 (4%)	0	100	100
13	К	140/142~(99%)	135 (96%)	5 (4%)	0	100	100
14	L	121/123~(98%)	117 (97%)	4 (3%)	0	100	100
15	М	142/144~(99%)	140 (99%)	2 (1%)	0	100	100
16	N	134/136~(98%)	131 (98%)	3 (2%)	0	100	100
17	Ο	123/127~(97%)	118 (96%)	5 (4%)	0	100	100
18	Р	115/117~(98%)	112 (97%)	3 (3%)	0	100	100
19	Q	112/115~(97%)	110 (98%)	2 (2%)	0	100	100
20	R	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
21	S	101/103~(98%)	99 (98%)	2 (2%)	0	100	100
22	Т	108/110~(98%)	105 (97%)	3 (3%)	0	100	100
23	U	93/100~(93%)	90 (97%)	3 (3%)	0	100	100
24	V	100/104~(96%)	99 (99%)	1 (1%)	0	100	100
25	W	92/94~(98%)	89 (97%)	3 (3%)	0	100	100
26	Х	74/85~(87%)	73 (99%)	1 (1%)	0	100	100
27	Y	75/78~(96%)	72 (96%)	3 (4%)	0	100	100
28	Z	60/63~(95%)	58 (97%)	2 (3%)	0	100	100
29	a	56/59~(95%)	55 (98%)	1 (2%)	0	100	100
30	b	54/57~(95%)	50 (93%)	4 (7%)	0	100	100
31	с	49/55~(89%)	48 (98%)	1 (2%)	0	100	100
32	d	44/46~(96%)	43 (98%)	1 (2%)	0	100	100
33	е	62/65~(95%)	59 (95%)	3(5%)	0	100	100
34	f	36/38~(95%)	36 (100%)	0	0	100	100
35	i	84/453~(18%)	84 (100%)	0	0	100	100
36	k	16/18~(89%)	12 (75%)	4 (25%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3532/4045~(87%)	3415~(97%)	115 (3%)	2~(0%)	50 79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	Н	118	PRO
11	Ι	108	VAL

#### 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	Perce	entiles
5	$\mathbf{C}$	216/218~(99%)	192 (89%)	24 (11%)	5	21
6	D	164/164~(100%)	154 (94%)	10~(6%)	15	41
7	Ε	165/165~(100%)	152 (92%)	13~(8%)	10	34
8	F	148/150~(99%)	130~(88%)	18 (12%)	4	19
9	G	137/138~(99%)	129~(94%)	8~(6%)	17	42
10	Н	114/114~(100%)	100 (88%)	14 (12%)	4	19
11	Ι	95/123~(77%)	89 (94%)	6~(6%)	15	40
12	J	104/110~(94%)	93~(89%)	11 (11%)	5	23
13	Κ	116/116~(100%)	105~(90%)	11 (10%)	7	26
14	L	104/104~(100%)	94 (90%)	10 (10%)	7	26
15	М	103/103~(100%)	94 (91%)	9~(9%)	8	30
16	Ν	109/109~(100%)	100 (92%)	9~(8%)	9	32
17	Ο	102/103~(99%)	95~(93%)	7~(7%)	13	37
18	Р	87/87~(100%)	75 (86%)	12 (14%)	3	17
19	Q	99/100~(99%)	90 (91%)	9~(9%)	7	28
20	R	89/90~(99%)	82 (92%)	7 (8%)	10	34
21	S	84/84~(100%)	76~(90%)	8 (10%)	7	26
22	Т	93/93~(100%)	88~(95%)	5(5%)	18	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentil	es
23	U	82/84~(98%)	77~(94%)	5~(6%)	15 41	]
24	V	83/85~(98%)	76~(92%)	7 (8%)	9 32	
25	W	78/78~(100%)	72 (92%)	6 (8%)	10 34	
26	Х	57/63~(90%)	51 (90%)	6 (10%)	5 23	
27	Y	67/68~(98%)	63 (94%)	4 (6%)	16 41	
28	Z	54/55~(98%)	47 (87%)	7 (13%)	3 18	
29	a	48/49~(98%)	46 (96%)	2(4%)	25 49	
30	b	47/48~(98%)	35~(74%)	12 (26%)	0 3	
31	с	45/49~(92%)	40 (89%)	5 (11%)	5 21	
32	d	38/38~(100%)	32~(84%)	6 (16%)	2 13	
33	е	51/52~(98%)	47 (92%)	4 (8%)	10 34	
34	f	34/34~(100%)	31 (91%)	3 (9%)	8 30	
35	i	71/341~(21%)	65~(92%)	6 (8%)	8 31	
36	k	17/17~(100%)	15 (88%)	2 (12%)	4 20	
All	All	2901/3232~(90%)	2635 (91%)	266 (9%)	10 28	

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5 of 266 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
30	b	18	SER
30	b	46	ASP
35	i	369	ASP
12	J	55	ILE
12	J	21	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
26	Х	46	HIS
35	i	411	GLN
28	Ζ	39	GLN
32	d	29	GLN
12	J	31	GLN

5.3.3 RNA (i)



Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	42/113~(37%)	13 (30%)	0
2	2	2/3~(66%)	1 (50%)	0
3	А	2878/2903~(99%)	518 (17%)	19~(0%)
4	В	119/120~(99%)	13 (10%)	0
All	All	3041/3139~(96%)	545 (17%)	19~(0%)

5 of 545 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	33	С
1	1	36	U
1	1	37	U
1	1	38	U
1	1	39	А

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type
3	А	2422	С
3	А	2602	А
3	А	2756	U
3	А	2430	А
3	А	1344	U

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

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

#### 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

#### 5.6 Ligand geometry (i)

Of 432 ligands modelled in this entry, 432 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers (i)

There are no such residues in this entry.

# 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-8004. 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: 144

Y Index: 144



Z Index: 144

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: 165

Y Index: 150

Z Index: 166

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 0.05. 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  $1693 \text{ nm}^3$ ; this corresponds to an approximate mass of 1530 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  $\text{\AA}^{-1}$ 



# 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-8004 and PDB model 5GAH. Per-residue inclusion information can be found in section 3 on page 11.

## 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.05 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 (0.05).



## 9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 91% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	$\mathbf{Q} extsf{-score}$
All	0.9090	0.3880
1	0.7850	0.1610
2	0.9360	0.4300
А	0.9530	0.3920
В	0.9820	0.3990
С	0.8470	0.4420
D	0.8660	0.4400
Е	0.8250	0.4010
F	0.8190	0.3330
G	0.8570	0.3810
Н	0.5880	0.2850
Ι	0.6240	0.1910
J	0.5320	0.1210
Κ	0.8750	0.4340
L	0.7960	0.4210
М	0.8590	0.4120
Ν	0.8560	0.4350
О	0.8470	0.4110
Р	0.8840	0.4000
Q	0.8260	0.4050
R	0.8740	0.4190
S	0.8770	0.4320
Т	0.8130	0.4270
U	0.8080	0.3860
V	0.8360	0.4030
W	0.8740	0.4250
Х	0.8650	0.4480
Y	0.8470	0.4240
Z	0.8020	0.3690
a	0.8700	0.4200
b	0.8390	0.4110
с	0.8180	0.3950
d	0.8650	0.4380
e	0.8720	0.4570
f	0.8800	0.4360

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Chain	Atom inclusion	Q-score
i	0.5820	0.2390
k	0.5330	0.1660

