

wwPDB EM Validation Summary Report (i)

Mar 13, 2024 – 01:23 PM JST

PDB ID 3J3V : EMDB ID : EMD-5642 Title : Atomic model of the immature 50S subunit from Bacillus subtilis (state I-a) Li, N.; Guo, Q.; Zhang, Y.; Yuan, Y.; Ma, C.; Lei, J.; Gao, N. Authors : Deposited on 2013-04-28 : 13.30 Å(reported) Resolution : Based on initial models 2J01, 2AW4 :

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.dev70
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

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 13.30 Å.

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



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM\ structures}\ (\#{ m Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain		
1	0	50	5%		
	0	59	86%	7% 7%	
2	2	44	93%	7%	
			18%		
3	5	232	44% 7% 48%	6	
			77%		
4	6	141	94%	6%	
5	А	2927	• 53% 36%	9% •	
			7%		
6	В	119	• 66%	25% 8%	
-	C	077	·		
(C	277	90%	9% •	

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Mol	Chain	Length	Quality of chain	
8	D	209	89%	9% ••
9	Е	207	● 86%	12% •
10	F	179	86%	13% •
11	G	179	87%	• 9%
12	J	145	86%	11% ••
13	K	122	93%	7%
14	L	146	85%	12% •
15	Ν	120	94%	6%
16	0	120	83%	15% •
17	Р	115	73%	20% • •
18	Q	119	94%	• • •
19	R	102	88%	11% •
20	S	113	93%	5% ••
21	Т	95	86%	12% •
22	U	103	84%	15% ·
23	Х	66	85%	8% 8%
24	Y	59	92%	• 5%

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2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 86157 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 50S ribosomal protein L32.

Mol	Chain	Residues		Atc	\mathbf{ms}	AltConf	Trace		
1	0	55	Total 433	C 267	N 87	0 72	${ m S} 7$	0	0

• Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues		Atc	\mathbf{ms}	AltConf	Trace		
2	2	44	Total 368	C 222	N 89	O 55	S 2	0	0

• Molecule 3 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues		At	oms	AltConf	Trace		
3	5	120	Total 910	C 576	N 156	0 176	${S \over 2}$	0	0

• Molecule 4 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues		At	oms	AltConf	Trace		
4	6	141	Total 1044	C 657	N 184	0 196	S 7	0	0

• Molecule 5 is a RNA chain called ribosome RNA 23S.

Mol	Chain	Residues		-	AltConf	Trace			
5	А	2884	Total 61914	C 27625	N 11428	O 19979	Р 2882	0	0

• Molecule 6 is a RNA chain called ribosome RNA 5S.

Mol	Chain	Residues		At	AltConf	Trace			
6	В	119	Total 2542	C 1135	N 462	0 827	Р 118	0	0



• Molecule 7 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues		Ate	AltConf	Trace			
7	С	277	Total 2129	C 1323	N 419	O 380	${f S}7$	0	0

• Molecule 8 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues		At	oms	AltConf	Trace		
8	D	206	Total 1568	C 984	N 289	O 290	${ m S}{ m 5}$	0	0

• Molecule 9 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues		At	oms	AltConf	Trace		
9	Е	206	Total 1567	C 983	N 290	O 292	${ m S} { m 2}$	0	0

• Molecule 10 is a protein called 50S ribosomal protein L5.

Total C N O S		
10 F 179 1413 898 246 261 8 0	10	0

• Molecule 11 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues		At	AltConf	Trace			
11	G	163	Total 1246	C 776	N 226	0 242	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

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

Mol	Chain	Residues		At	AltConf	Trace			
12	J	143	Total	C 717	N 207	0	S 6	0	0
			1154	(1)	207	204	0		

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

Mol	Chain	Residues		At	AltConf	Trace			
13	К	122	Total 921	C 571	N 173	0 173	${S \atop 4}$	0	0

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



Mol	Chain	Residues		At	oms			AltConf	Trace
14	L	146	Total 1082	C 671	N 207	O 202	${ m S} { m 2}$	0	0

• Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues		At	oms	AltConf	Trace		
15	Ν	120	Total 962	C 588	N 187	0 182	${ m S}{ m 5}$	0	0

• Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues		At	AltConf	Trace			
16	О	120	Total 913	С 564	N 176	0 172	S 1	0	0

• Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
17	P	119	Total	С	Ν	Ο	0	0
11	1	112	916	584	178	154	0	0

• Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues		At	AltConf	Trace			
18	Q	117	Total 940	C 591	N 189	O 156	S 4	0	0

• Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues		At	oms	AltConf	Trace		
19	R	102	Total 795	C 506	N 140	0 148	S 1	0	0

• Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues		At	oms	AltConf	Trace		
20	S	112	Total 868	C 541	N 168	0 155	${S \atop 4}$	0	0

• Molecule 21 is a protein called 50S ribosomal protein L23.



Mol	Chain	Residues		At	oms			AltConf	Trace
21	Т	95	Total 767	C 480	N 139	0 144	$\frac{S}{4}$	0	0

• Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues		At	oms		AltConf	Trace	
22	U	103	Total 780	C 488	N 145	0 143	$\frac{S}{4}$	0	0

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

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
23	Х	61	Total 504	C 312	N 97	O 93	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

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

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
24	Y	56	Total	С	N	0	S	0	0
			441	273	86	81	1		



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: 50S ribosomal protein L32







E140 D141

• Molecule 5: ribosome RNA 23S







G721	A722 A723	A724	C725	C726 A727	G728	G729	0/30 G731	A732	U733	C/34 11735	A736	C737	C738	0139 A740	U741	G742	0744 C744	C745	A746	6748 6748	G749	U750	G751	A752 A753	G754	U755	U756 C757	A758	G759	G760 11761	A762	A763	C764	C766	U767	A769	A770	U771	G773	A774	G775	G777 C777	C778	<mark>C779</mark> G780	
A781	A782 C783	C784	C785	A786 C787	G788	C789	A/ 90 C791	G792	U7 93	0794 C795	A796	A797	A7 98	A/ 33 G800	U801	G802	G804	G805	G806	6807 A808	U809	G810	A811	G812 C813	U814	G815	0816 G817	G818	G819	U820 4821	G822	G823 G824	G825	U826	4828	A829	A830	0031 G832	C833	C834	A835 A836	U837	C838	4840	
A841	C842 C843	U844	G845	G846 A847	G848	A849	0650 A851	G852	C853	0854 C855	G856	U857	1858 7050	0980	C861	U862	C864 C864	G865	A866	A867 A868	U869	A870	G871	C872	00/3 U874	U875	A876 G877	G878	G879	C880	4882	G883	C004 C885	U886 0007	4888	A889	G890	1892	A893	A894	6895 A896	G897	0898 7000	006N	
01	03	04	05	06	80	60	11	12	13	14	16	17	18	20	21	22	24	125	26	27	29	30	31	32	33	34	35	36	38	39	140	42	143 1	45	46)47 10	048 049	50	51	52	54	55	57	20	09
5D		AG	55		AG	55	GG	50	AG		3 23	AG		200	59	AG		AS	SB	55 0	3 33	S	SC	SS	S	50	AG	88	2 29	55	00	50	AS		55	AS	AS UC	SN	8	AC CC	50	5	AS	AG	50
C961	C962 C963	A964	A965	0966 0967	C968	C969	A971 A971	U972	G973	A9/4 7075	U976	77 0 0	A978	0979 7000	C981	U982	0983 0084	0605 0985	G986	A987	1080	0660	A991	G992	A993 Cool	1995	966D	1997 1998	A999	G1000	01001 61002	A1003	U1004 A1005	A1006	G1007	011009 U1009	C1010	C1011	U1012	A1014	G1015	01010 C1017	G1018	A1019 A1020	
A1021	61022	G1024	A1025	A1026 A1027	C1028	A1029	G1031	<mark>C1032</mark>	C1033	A1034	A1036	C1037	C1038	G1040	C1041	A1042	G1043 C1044	U1045	A1046	A1047	G1049	<mark>U1050</mark>	C1051	C1052	A1054	A1055	A1056 G1057	U1058	A1059	U1060 41061	C1062	G1063	U1065	A1066	G1068	U1069	G1070	A1072	A1073	A1074	A1075 G1076	G1077	A1078	01079 G1080	
081	082	084	085	086	088	089 089	091	092	093	094	0960	097	038	000	101	102	103 104	10 1 105	106	107	108 100	110	111	112	113	115 115	116	117	118	120	121	122 123	124	125 176	127	128	129	130	131 132	133 133	134	135 136	137	138 139	140
U1	55	A1	G1	55	5	<mark>5</mark> 8		A1	5	A1 F	A1	A1	C1		15 15	G	A1	610	11	U1	5 5	50	U1	U	A1	G1 A1	A1	61	C1 A1	15	C1		C1	C1		10	U1	A1		61	A1	01 11	61	<mark>5 5</mark>	11
A1141	A1142	A1144	G1145	C1146	0114/ C1148	A1149	C1150	G1152	G1153	U1154	C1155	A1157	G1158	01159 01160	A1161	C1162	U1163	0110 1 01165	G1166	C1167	G1168	C1170	G1171	A1172	A1173 A117A	A1175	U1176	G1177	A1179	C1180	C1181 G1182	G1183	G1184 C1185	C1186	U1187	A1100 A1189	A1190	C1191	U1193	A1194	U1195	01190 A1197	C1198	C1199 G1200	
A1201	A1202	C1204	U1205	G1206 C1207	G1208	G1209	A1210 C1211	U1212	G1213	01214 11215	C1216 C1216	U1217	U1218	G1219 G1220	A1221	A1222	C1 223 A1 224	G1225	U1226	G1227 C1228	01229	A1230	G1231	G1232 A1233	61234 G1234	A1235	G1236 C1237	G1238	U1239	01240 C1241	01242 U1242	A1243	A1 244 G1 245	G1246	G1 248 C1 248	U1249	G1250	01251 G1252	A1253	A1254	G1256 C1256	C1257	A1258	A1260	
C1261	C1262 C1263	G1264	A1265	A1266 G1267	G1268	A1269	U1271	G1272	G1273	01274 01275	G1276	A1277	G1278	G1280	C1281	U1282	01283 A1284	<mark>G1285</mark>	A1286	A1287	U1289	<mark>G1290</mark>	A1291	G1292 A1203	A1294	<mark>U1295</mark>	G1296	C1298	G1299	G1300	A1302	U1303	A1305	G1306	A1308	G1309	<mark>C1310</mark>	A1312	A1313	A1314	G1315	A1316 G1317	<mark>G1318</mark>	<mark>G1319</mark> G1320	
U1321	G1322 A1323	G1324	A1325	A1326 111327	C1328	C1329	C1330 C1331	<mark>U1332</mark>	C1333	C1334 A1335	C1336	<mark>C1337</mark>	G1338 A1230	A1339 A1340	U1341	G1342	C1343 C1344	U1345	A1346	A1347 C1348	G1349	U1350	U1351	01352 C1353	C1354	U1355	G1356 A1357	G1358	G1359	A1360 A1361	G1362	G1363 G1363	01365 U1365	C1366	U1368	C1369	C1370	G1371 C1372	<mark>U1373</mark>	C1374	A1375 G1376	G1377	G1378 111 270	01380	
A1381	G1382	C1384	G1385	G1386 G1387	A1388	C1389	U1391	A1392	A1393	G1394	C1396	G1397	A1398	G1400	C1401	C1402	61403 A1404	A1405	A1406	G1407	C1409	G1410	U1411	A1412 61413	G1414	C1415	G1416 A1417	U1418	G1419	G1420 A1421	C1422	A1423	A1425 C1425	A1426	G1428	U1429	U1430	41431 A1432	U1433	A1434	U1435 U1436	C1437	C1438	G1440	
U1441	A1442	C1444	A1445	C1446 C1447	U1448	C1449	01450 U1451	C1452	A1453	C1454 C1455	A1456	U1457	U1458 111450	01453 G1460	A1461	G1462	C1463 A1464	A1465	U1466	G1467	G1469	G1470	G1471	G1472	C1474	G1475	C1476 A1477	G1478	G1479	A1480 C1481	G1482	A1483	01404 A1485	G1486	G1488	U1489	A1490	G1492	C1493	G1494	G1495 G1496	G1497	U1498	U1500	
U1501	G1502 G1503	A1504	U1505	A1506 111507	C1508	C1509	C1511	G1512	01513	C1514 C1515	A1516	A1517	G1518 C1518	01519 A1520	G1521	U1522	01523 A1524	G1525	G1526	C1527 111578	G1529	G1530	G1531	A1532 A1533	A1534	U1535	A1536 C1537	G1538	C1539	A1540 A1541	A1542	U1543	C1545	G1546	01347 U1548	U1549	C1550	C1552	A1553	U1554	A1555	A 1930 G 1557	G1558	C1559 U1560	





PROTEIN DATA BANK









• Molecule 21: 50S rib	posomal protein L23	
Chain T:	86%	12% ·
M1 82 83 85 85 86 86 86 86 86 86 86 86 86 86 86 86 86	T70 170 885 887 887 887 887 887 887	
• Molecule 22: 50S rib	posomal protein L24	
Chain U:	84%	15% •
M1 K6 K8 K8 K15 K15 A25 A25 A25 A25 A25 A25	K42 K43 H44 P47 P47 P47 G53 G54 G54 G55 G55 G55 G55 G55 G55 G55 G55	
• Molecule 23: 50S rib	posomal protein L29	
Chain X:	85%	8% 8%
M1 E15 E15 E15 E15 E15 E16 E14 E11 E11 E11 E11 E11 E11 E11 E11 E11	LYS	
• Molecule 24: 50S rib	oosomal protein L30	
17%		
Chain Y:	92%	• 5%
MET ALA ALA ALA ALA ALA Case Case Case Case Case Case Case Case	135 H152 K57 €58 GLN	



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	21020	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	20	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	59000	Depositor
Image detector	FEI EAGLE $(4k \times 4k)$	Depositor
Maximum map value	10.841	Depositor
Minimum map value	-4.301	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.7	Depositor
Map size (Å)	384.0, 384.0, 384.0	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.5, 1.5, 1.5	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	B	ond lengths		Bond angles
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
1	0	1.04	0/440	1.06	1/584~(0.2%)
2	2	1.26	0/371	1.06	0/483
3	5	0.87	0/921	1.10	1/1239~(0.1%)
4	6	0.91	0/1058	1.02	0/1427
5	А	1.69	134/69349~(0.2%)	2.70	8798/108189~(8.1%)
6	В	1.64	4/2843~(0.1%)	2.64	336/4432~(7.6%)
7	С	1.01	0/2166	1.09	2/2902~(0.1%)
8	D	0.96	0/1590	1.07	0/2130
9	Ε	0.97	0/1586	1.08	2/2139~(0.1%)
10	F	0.96	0/1432	1.09	2/1920~(0.1%)
11	G	0.98	0/1264	1.05	0/1709
12	J	0.94	0/1157	1.04	0/1557
13	Κ	1.03	0/928	1.05	0/1245
14	L	0.98	0/1094	1.09	2/1457~(0.1%)
15	Ν	1.08	0/969	1.06	0/1294
16	0	1.01	0/922	1.05	1/1236~(0.1%)
17	Р	1.10	0/929	1.21	5/1243~(0.4%)
18	Q	1.06	0/952	1.08	4/1266~(0.3%)
19	R	0.91	0/806	1.09	0/1080
20	S	1.01	0/877	1.13	1/1179~(0.1%)
21	Т	1.00	0/774	1.11	1/1030~(0.1%)
22	U	0.87	0/790	1.15	0/1054
23	Х	1.05	0/505	1.02	0/671
24	Y	0.97	0/443	1.01	0/594
All	All	1.55	138/94166~(0.1%)	2.45	9156/142060~(6.4%)

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	А	0	447

Continued on next page...



Mol	Chain	#Chirality outliers	#Planarity outliers
6	В	0	15
8	D	0	2
9	Ε	0	1
14	L	0	2
15	N	0	1
17	Р	0	3
21	Т	0	3
All	All	0	474

Continued from previous page...

The worst 5 of 138 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	А	1253	A	N7-C5	-7.44	1.34	1.39
5	А	353	А	N7-C5	-7.42	1.34	1.39
5	А	629	G	C2'-C1'	-7.08	1.45	1.53
5	А	1449	С	P-O5'	-7.08	1.52	1.59
5	А	2297	А	N7-C5	-6.86	1.35	1.39

The worst 5 of 9156 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	В	10	G	P-O3'-C3'	26.30	151.26	119.70
5	А	1339	A	P-O3'-C3'	26.04	150.94	119.70
5	А	178	А	P-O3'-C3'	22.26	146.41	119.70
5	А	2062	А	P-O3'-C3'	21.01	144.91	119.70
5	А	74	U	P-O3'-C3'	20.60	144.42	119.70

There are no chirality outliers.

5 of 474 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	А	14	A	Sidechain
5	А	15	G	Sidechain
5	А	27	G	Sidechain
5	А	28	А	Sidechain
5	А	3	U	Sidechain

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



Mol	Chain	Non-H	${ m H}({ m model})$	H(added)	Clashes	Symm-Clashes
1	0	433	0	454	0	0
2	2	368	0	410	0	0
3	5	910	0	944	2	0
4	6	1044	0	1098	1	0
5	А	61914	0	31166	148	0
6	В	2542	0	1288	6	0
7	С	2129	0	2225	0	0
8	D	1568	0	1635	2	0
9	Е	1567	0	1652	3	0
10	F	1413	0	1479	2	0
11	G	1246	0	1273	0	0
12	J	1134	0	1178	3	0
13	Κ	921	0	977	0	0
14	L	1082	0	1132	3	0
15	Ν	962	0	995	0	0
16	0	913	0	947	4	0
17	Р	916	0	987	2	0
18	Q	940	0	1005	1	0
19	R	795	0	838	0	0
20	S	868	0	930	0	0
21	Т	767	0	813	0	0
22	U	780	0	838	1	0
23	Х	504	0	541	0	0
24	Y	441	0	478	0	0
All	All	86157	0	55283	174	0

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.

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 1.

The worst 5 of 174 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)
5:A:1799:G:H1	5:A:2011:U:H3	1.32	0.76
5:A:2557:U:H3	5:A:2564:A:H61	1.39	0.68
5:A:1672:A:H61	5:A:1684:U:H3	1.43	0.65
5:A:1339:A:C2	5:A:1679:A:C2	2.87	0.62
5:A:1976:C:H2'	5:A:1977:G:H5"	1.80	0.62

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	Per	$\operatorname{centiles}$
1	0	53/59~(90%)	40 (76%)	10 (19%)	3 (6%)	1	18
2	2	42/44~(96%)	38~(90%)	2~(5%)	2(5%)	2	21
3	5	116/232~(50%)	96 (83%)	11 (10%)	9 (8%)	1	13
4	6	139/141 (99%)	117 (84%)	15 (11%)	7 (5%)	2	20
7	С	275/277~(99%)	224 (82%)	33 (12%)	18 (6%)	1	16
8	D	204/209~(98%)	158 (78%)	38 (19%)	8 (4%)	3	23
9	Е	204/207~(99%)	166 (81%)	19 (9%)	19 (9%)	0	11
10	F	177/179~(99%)	136 (77%)	27 (15%)	14 (8%)	1	13
11	G	161/179~(90%)	150 (93%)	9 (6%)	2 (1%)	13	3 50
12	J	141/145~(97%)	117 (83%)	14 (10%)	10 (7%)	1	14
13	К	120/122~(98%)	103 (86%)	11 (9%)	6 (5%)	2	20
14	L	144/146~(99%)	105 (73%)	24 (17%)	15 (10%)	() 8
15	N	118/120 (98%)	96 (81%)	19 (16%)	3 (2%)	5	32
16	Ο	118/120 (98%)	87 (74%)	18 (15%)	13 (11%)	() 7
17	Р	110/115~(96%)	71 (64%)	23 (21%)	16 (14%)	() 4
18	Q	115/119~(97%)	104 (90%)	10 (9%)	1 (1%)	17	7 57
19	R	100/102~(98%)	79 (79%)	13 (13%)	8 (8%)	1	12
20	S	110/113~(97%)	97 (88%)	8 (7%)	5 (4%)	2	22
21	Т	93/95~(98%)	70 (75%)	14 (15%)	9 (10%)	0	10
22	U	101/103 (98%)	71 (70%)	18 (18%)	12 (12%)	() 6
23	X	59/66~(89%)	53 (90%)	4 (7%)	2 (3%)	3	26
24	Y	54/59~(92%)	47 (87%)	5 (9%)	2 (4%)	3	24
All	All	2754/2952 (93%)	2225 (81%)	345 (12%)	184 (7%)	2	15

5 of 184 Ramachandran outliers are listed below:



Mol	Chain	Res	Type
3	5	41	THR
3	5	209	VAL
3	5	212	VAL
4	6	93	ASN
7	С	34	LEU

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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	0	49/53~(92%)	49 (100%)	0	100	100
2	2	39/39~(100%)	38~(97%)	1 (3%)	46	66
3	5	98/185~(53%)	93~(95%)	5(5%)	24	48
4	6	110/110 (100%)	110 (100%)	0	100	100
7	С	225/225~(100%)	213 (95%)	12 (5%)	22	47
8	D	167/170~(98%)	157 (94%)	10 (6%)	19	44
9	Е	169/170~(99%)	163 (96%)	6 (4%)	35	59
10	F	154/154~(100%)	147 (96%)	7 (4%)	27	52
11	G	138/151~(91%)	133 (96%)	5 (4%)	35	59
12	J	122/123~(99%)	113 (93%)	9~(7%)	13	38
13	K	101/101 (100%)	98~(97%)	3 (3%)	41	63
14	L	110/110 (100%)	107 (97%)	3(3%)	44	65
15	Ν	100/100 (100%)	97~(97%)	3 (3%)	41	63
16	Ο	93/93~(100%)	90~(97%)	3(3%)	39	61
17	Р	97/100~(97%)	90~(93%)	7 (7%)	14	39
18	Q	96/98~(98%)	95~(99%)	1 (1%)	76	86
19	R	84/84~(100%)	79~(94%)	5~(6%)	19	44
20	S	93/93~(100%)	91~(98%)	2(2%)	52	71
21	Т	85/85~(100%)	83 (98%)	2(2%)	49	69
22	U	87/87~(100%)	84 (97%)	3 (3%)	37	60

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Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles	;
23	Х	54/57~(95%)	51 (94%)	3~(6%)	21	46	
24	Y	51/53~(96%)	51 (100%)	0	100	100	
All	All	2322/2441~(95%)	2232 (96%)	90 (4%)	36	56	

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5 of 90 residues with a non-rotameric side chain are listed below:

Mol	Chain	\mathbf{Res}	Type
13	Κ	90	ASP
17	Р	74	PHE
14	L	51	GLU
16	0	94	VAL
19	R	10	LYS

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such side chains are listed below:

Mol	Chain	Res	Type
16	0	103	HIS
20	S	2	GLN
10	F	37	ASN
10	F	172	GLN
11	G	23	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	А	2882/2927~(98%)	895~(31%)	205~(7%)
6	В	118/119~(99%)	24 (20%)	3(2%)
All	All	3000/3046~(98%)	919~(30%)	208~(6%)

5 of 919 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	А	2	G
5	А	3	U
5	А	4	U
5	А	8	U
5	А	10	А

5 of 208 RNA pucker outliers are listed below:



Mol	Chain	Res	Type
5	А	1606	А
5	А	1999	А
5	А	2870	G
5	А	1629	С
5	А	1787	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-5642. 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: 128



Y Index: 128



Z Index: 128



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: 143

Y Index: 139

Z Index: 130

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 2.7. 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 1820 nm^3 ; this corresponds to an approximate mass of 1644 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 0.075 ${\rm \AA^{-1}}$



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-5642 and PDB model 3J3V. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 2.7 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 (2.7).



9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 92% 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 (2.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9230	0.0810
0	0.9480	0.0410
2	1.0000	0.0160
5	0.6230	0.0580
6	0.2030	0.0410
А	0.9360	0.0910
В	0.8530	0.0870
С	0.9600	0.0350
D	0.9660	0.0560
Е	0.9690	0.0560
F	0.8480	0.0720
G	0.8840	0.0820
J	0.9580	0.0420
K	0.9360	0.0590
L	0.9120	0.0420
Ν	1.0000	0.0510
0	0.9280	0.0730
Р	0.9120	0.0450
Q	0.9670	0.0250
R	0.9800	0.0700
S	0.9680	0.0470
Т	0.9910	0.0490
U	0.9550	0.0470
Х	0.9920	0.0830
Y	0.7490	0.0410

