

wwPDB EM Validation Summary Report (i)

Jun 13, 2022 – 08:06 pm BST

PDB ID	:	7QGR
EMDB ID	:	EMD-13958
Title	:	Structure of the SmrB-bound E. coli disome - collided 70S ribosome
Authors	:	Kratzat, H.; Buschauer, R.; Berninghausen, O.; Beckmann, R.
Deposited on	:	2021-12-09
Resolution	:	5.70 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 following versions of software and data (see references (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1. dev 8
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

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 5.70 Å.

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



Metric	Whole archive	EM structures
	(#Entries)	(#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	Ο	120	25%	19% ••
2	Р	273	72% 87%	10% ••
3	Q	209	65% 93%	7%
4	R	201	59% 95%	
5	S	179	85%	•••
6	Т	177	87%	. .
7	V	142	93%	
8	W	142	49% 95%	5%



Mol	Chain	Length	Quality of chain	
9	X	123	80%	
		120	65%	·
10	Υ	144	89%	8% ••
11	7	100	60%	
11	Z	136	90%	9% •
12	a	127	83%	10% . 6%
			72%	10/0 0 0/0
13	b	117	94%	5%•
14		115	76%	
14	с	115	92%	5% ••
15	Ь	118	88%	10%
10	u	110	73%	1070 ••
16	е	103	95%	• •
	c	110	71%	
17	t	110	97%	•
18	σ	100	10%	70/
10	6	100	56%	• /%
19	h	104	94%	
			45%	
20	i	94	100%	
21	i	85	18%	F0/ 120/
21	J	00	59%	5% • 12%
22	k	78	92%	6% •
			70%	
23	1	63	94%	6%
24	m	50	46%	
24	111	- 09	42%	• •
25	n	57	82%	16% •
			69%	
26	0	55	85%	5% 9%
97	n	46	57%	1.00/
21	р	40	46%	13%
28	q	65	88%	9% ••
	1		49%	
29	r	55	60% 9%	31%
20	N	2002	15%	2004
- 30	LΝ	2900	66% 77%	29% 5%
31	\mathbf{L}	70	76%	• 23%
			60%	
32	С	223	60%	40%
20	TT	140	99%	
აპ	U	149	98%	·



Mol	Chain	Length	Quality of chain	
			63%	
34	М	75	81%	19%
35	х	692	••••• 94%	
2.6	0	1 - 00	·	
36	0	1539	72%	25% •
37	1	239	87%	• 9%
			62%	
38	2	218	90%	• 6%
39	3	206	98%	·
			65%	
40	4	162	83%	9% • 7%
41	5	131	66% 10%	24%
			50%	
42	6	152	97%	••
43	7	130	47%	
10	•	100	59%	••
44	8	130	88%	8% ••
45	0	103	62%	F0(F0(
40	3	105	64%	5% • 5%
46	А	129	87%	• 9%
17	В	194	48%	70/
41	D	124	<u> </u>	/% ••
48	D	118	90%	6% • •
40	д	101	57%	
49	Ē	101	36%	7% 5%
50	F	89	91%	7% ••
۳1	C	00	41%	
51	G	82	94%	6%
52	Н	84	88%	7% 5%
50	т	Ĩ	36%	
53	1	75	68% 5%	27%
54	J	92	83%	•• 14%
	τ.		44%	
55	К	87	93%	• • •
56	S	71	66% • •	28%
			26%	
57	t	557	25% • 74%	
58	u	73	73%	27%



Mol	Chain	Length	Quality of chain	
			74%	
59	V	182	92%	••• •



2 Entry composition (i)

There are 62 unique types of molecules in this entry. The entry contains 149850 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 5S rRNA.

Mol	Chain	Residues	Atoms				AltConf	Trace	
1	Ο	118	Total 2529	C 1126	N 464	0 821	Р 118	0	0

• Molecule 2 is a protein called 50S ribosomal protein L2.

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

• Molecule 3 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	209	Total 1564	C 979	N 288	O 293	${S \atop 4}$	0	0

• Molecule 4 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms				AltConf	Trace	
4	R	201	Total 1552	C 974	N 283	O 290	${ m S}{ m 5}$	0	0

• Molecule 5 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms				AltConf	Trace	
5	S	177	Total 1397	C 891	N 249	0 251	S 6	0	0

• Molecule 6 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues		At	AltConf	Trace			
6	Т	176	Total 1322	C 832	N 243	0 245	${S \over 2}$	0	0



• Molecule 7 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues		At	oms			AltConf	Trace
7	V	141	Total 1031	C 651	N 179	0 195	S 6	0	0

• Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	W	142	Total 1128	С 714	N 212	0 198	$\frac{S}{4}$	0	0

• Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues		At	oms			AltConf	Trace
9	Х	122	Total 938	C 587	N 180	0 165	S 6	0	0

• Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues		At	AltConf	Trace			
10	Y	143	Total 1044	C 649	N 206	0 188	S 1	0	0

• Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues		At	oms			AltConf	Trace
11	Z	136	Total 1073	C 686	N 205	0 176	S 6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	a	120	Total 960	C 593	N 196	0 166	${ m S}{ m 5}$	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	123	ALA	GLU	conflict	UNP A0A829CNM8

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



Mol	Chain	Residues		Ato	ms		AltConf	Trace
13	b	116	Total 891	C 552	N 178	O 161	0	0

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

Mol	Chain	Residues		At	oms			AltConf	Trace
14	с	114	Total 915	C 573	N 179	0 162	S 1	0	0

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

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace	
15	d	117	Total 946	C 604	N 192	O 150	0	0

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

Mol	Chain	Residues		At	oms			AltConf	Trace
16	е	103	Total 815	C 516	N 153	0 144	${ m S} { m 2}$	0	0

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

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

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

Mol	Chain	Residues		At	oms			AltConf	Trace
18	g	93	Total 738	C 466	N 139	0 131	${ m S} { m 2}$	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	98	SER	GLY	conflict	UNP A0A829CFV1

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



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

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

Mol	Chain	Residues		At	oms			AltConf	Trace
20	i	94	Total 752	C 479	N 137	0 133	${ m S} { m 3}$	0	0

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

Mol	Chain	Residues		At	oms			AltConf	Trace
21	j	75	Total 568	C 353	N 113	0 101	S 1	0	0

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

Mol	Chain	Residues		At	oms			AltConf	Trace
22	k	77	Total 624	C 388	N 129	0 105	${ m S} { m 2}$	0	0

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

Mol	Chain	Residues		Ato	\mathbf{ms}			AltConf	Trace
23	1	63	Total 508	C 313	N 99	0 94	S 2	0	0

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

Mol	Chain	Residues		Ato	\mathbf{ms}			AltConf	Trace
94	m	59	Total	С	Ν	Ο	S	0	0
24	111	- 10	448	281	87	78	2	0	0

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

Mol	Chain	Residues		Atc	\mathbf{ms}			AltConf	Trace
25	n	56	Total 443	C 269	N 94	O 79	S 1	0	0

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



Mol	Chain	Residues		Aton	ns		AltConf	Trace
26	0	50	Total 409	C 263	N 75	O 71	0	0

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

Mol	Chain	Residues		Ato	\mathbf{ms}			AltConf	Trace
27	р	46	Total 376	C 228	N 90	O 56	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

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

Mol	Chain	Residues		At	oms			AltConf	Trace
28	q	64	Total 503	C 323	N 105	O 73	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

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

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
29	r	38	Total 201	C 185	N 65	0 47	S 4	0	0
			301	100	05	41	4		

• Molecule 30 is a RNA chain called 23S rRNA.

Mol	Chain	Residues			AltConf	Trace			
30	Ν	2897	Total 62215	C 27754	N 11448	O 20115	Р 2898	1	0

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

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
31	T.	54	Total	С	Ν	Ο	S	0	Ο
51	Ľ	04	415	256	75	78	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	68	SER	GLY	conflict	UNP A0A1X3HZV8

• Molecule 32 is a protein called 50S ribosomal protein L1.



Mol	Chain	Residues		At	oms			AltConf	Trace
32	С	134	Total 1027	$\begin{array}{c} \mathrm{C} \\ 645 \end{array}$	N 186	0 194	${ m S} { m 2}$	0	0

• Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues		At	oms	AltConf	Trace		
33	U	149	Total 1111	C 699	N 197	0 214	S 1	0	0

• Molecule 34 is a RNA chain called P-site tRNA.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
34	М	75	Total 1594	С 711	N 281	O 527	Р 75	0	0

• Molecule 35 is a RNA chain called mRNA.

Mol	Chain	Residues		At	toms			AltConf	Trace
35	х	44	Total 928	C 416	N 160	O 308	Р 44	0	0

• Molecule 36 is a RNA chain called 16S rRNA.

Mol	Chain	Residues		1	AltConf	Trace			
36	0	1539	Total 33015	C 14725	N 6052	O 10699	Р 1539	0	0

• Molecule 37 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues		Ate	AltConf	Trace			
37	1	218	Total 1699	C 1078	N 303	0 311	${ m S} 7$	0	0

• Molecule 38 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues		At	oms			AltConf	Trace
38	2	206	Total 1624	C 1028	N 305	0 288	${ m S} { m 3}$	0	0

• Molecule 39 is a protein called 30S ribosomal protein S4.



Mol	Chain	Residues	Atoms				AltConf	Trace	
39	3	205	Total 1642	C 1026	N 315	O 297	$\frac{S}{4}$	0	0

• Molecule 40 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	4	150	Total 1105	C 687	N 211	0 201	S 6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	4	MET	ILE	conflict	UNP A0A377C6M5

• Molecule 41 is a protein called 30S ribosomal protein S6, non-modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	5	100	Total 817	C 515	N 148	0 148	S 6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	101	SER	PRO	$\operatorname{conflict}$	UNP P02358

• Molecule 42 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	6	151	Total 1181	C 735	N 227	O 215	${S \atop 4}$	0	0

• Molecule 43 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	7	129	Total 978	C 616	N 173	0 183	S 6	0	0

• Molecule 44 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	8	127	Total 1021	C 634	N 206	0 178	${ m S} { m 3}$	0	0



There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
8	3	ASP	GLU	$\operatorname{conflict}$	UNP A0A1Z3UZ18

• Molecule 45 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	9	98	Total 786	C 493	N 150	0 142	S 1	0	0

• Molecule 46 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	А	117	Total 876	C 540	N 174	0 159	${ m S} { m 3}$	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	ALA	PRO	conflict	UNP A0A829AF87

• Molecule 47 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues		At	\mathbf{oms}			AltConf	Trace
47	В	123	Total 954	C 590	N 196	0 164	S 4	0	0

• Molecule 48 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues		At	oms			AltConf	Trace
48	D	114	Total 877	С 543	N 175	0 156	${ m S} { m 3}$	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	VAL	MET	conflict	UNP A0A7U9IV78

• Molecule 49 is a protein called 30S ribosomal protein S14.



Mol	Chain	Residues		At	oms			AltConf	Trace
49	Е	96	Total 773	C 483	N 160	0 127	${ m S} { m 3}$	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	40	ALA	GLU	conflict	UNP A0A090BZT4

• Molecule 50 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues		At	oms			AltConf	Trace
50	F	88	Total 709	C 437	N 143	0 128	S 1	0	0

• Molecule 51 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues		At	oms			AltConf	Trace
51	G	82	Total 648	C 406	N 128	0 113	S 1	0	0

• Molecule 52 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues		At	oms			AltConf	Trace
52	Н	80	Total 648	C 411	N 121	0 113	${ m S} { m 3}$	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Н	2	ALA	THR	conflict	UNP A0A829A8C6

• Molecule 53 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues		Aton	ıs		AltConf	Trace
53	Ι	55	Total 455	C 288	N 86	0 81	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ι	15	THR	ALA	conflict	UNP A0A376I7P4
Ι	58	ALA	CYS	conflict	UNP A0A376I7P4



• Molecule 54 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues		At	oms			AltConf	Trace
54	J	79	Total 637	C 408	N 120	O 107	${S \over 2}$	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	82	TYR	GLY	conflict	UNP S1EA57
J	83	TYR	HIS	conflict	UNP S1EA57

• Molecule 55 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace	
55	K	85	Total 664	C 411	N 137	0 113	${ m S} { m 3}$	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1	LEU	MET	conflict	UNP P0A7U7

• Molecule 56 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms				AltConf	Trace	
56	s	51	Total 425	C 265	N 86	O 73	S 1	0	0

• Molecule 57 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms			AltConf	Trace	
57	t	143	Total 704	C 418	N 143	0 143	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
t	241	VAL	ILE	conflict	UNP A0A829CYC5

• Molecule 58 is a RNA chain called A-site tRNA.



Mol	Chain	Residues	Atoms				AltConf	Trace	
58	u	73	Total 1561	$\begin{array}{c} \mathrm{C} \\ 695 \end{array}$	N 279	O 514	Р 73	0	0

• Molecule 59 is a protein called UPF0115 protein YfcN.

Mol	Chain	Residues	Atoms				AltConf	Trace	
59	v	175	Total 1256	C 796	N 226	0 229	${ m S}{ m 5}$	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	99	ALA	ASP	conflict	UNP Q6KCY1
V	101	ALA	HIS	conflict	UNP Q6KCY1

• Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
60	u	2	Total Mg 2 2	0

• Molecule 61 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
61	u	1	Total K 1 1	0

• Molecule 62 is water.

Mol	Chain	Residues	Atoms	AltConf
62	u	9	Total O 9 9	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: 5S rRNA



 \bullet Molecule 2: 50S ribosomal protein L2



 \bullet Molecule 3: 50S ribosomal protein L3

Chain Q:

93%

65%

7%















• Molecule 19: 50S ribosomal protein L24





• Molecule 25: 50S ribosomal protein L32











PROTEIN DATA BANK





V61 L62 A63 A64 A65 A65 A65 A67 A67 A69 E70 K71 Y72 N73 A74 A74 A74 C75	E76 177 V78 179 180 881 882 882 882 685 685 685 585 585 585 585 585 585	688 K89 F91 692 692 893 695 796 R95 R97 R97	D98 199 A100 A100 A102 V103 T104 A105 A105	V105 E109 V110 A111 K112 S113 E114 V115 F114 V115 P118 P118 C117 P118
121 122 123 123 125 125 125 125 125 125 123 123 123 123 123 123	1136 1137 1138 1139 1140 1141 1142 1145	11448 11449		
• Molecule 34: P-site tRN	Â			
Chain M:	63% 81%		19%	
U1 G2 G3 G4 G5 G5 G5 G5 C3 C3 C3 C3 C1 C11 C12 C11 C12 C12 C15 C15 C15	C16 G17 G17 G18 A20 C24 G42 G42 A44 A44 A44 C43 C47 C47 C47	48 49 450 451 452 452 453 455 455 457	A58 U59 C60 C61 U62 C63 C63 C63 C63 C63 C63	C C C C C C C C C C C C C C C C C C C
• Molecule 35: mRNA				
Chain x: •••	94%			
4 4 7 7 4 7 4 7 4 7 7 7 7 7 7 7 7 7 7 7	0 0 4 0 4 D 4 D A D 4 D 0 0 0 0 4 0 4 D 4 D 4 D 4 D 0 0	99999440440900 94004004004004	00000000000000000000000000000000000000	
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	< < < 0 U U U U G < < < 0 U			
• Molecule 36: 16S rRNA	720/	75	96	
	12%	25	•	





 \bullet Molecule 37: 30S ribosomal protein S2





• Molecule 40: 30S ribosomal protein S5



• Molecule 44: 30S ribosomal protein S9













ASN PHE SER ASN ASN ALA ALA ALA ALA ALA PHE LYS ALA ALA ALA ALA ALA ALA CLY CLY





• Molecule 59: UPF0115 protein YfcN





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32412	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 $(e^-/\text{\AA}^2)$	42.4	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.070	Depositor
Minimum map value	-0.867	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.081	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	847.19995, 847.19995, 847.19995	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.412, 1.412, 1.412	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: MG, K

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	1	Bond angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	0	0.80	1/2828~(0.0%)	0.88	6/4410~(0.1%)
2	Р	1.41	22/2121~(1.0%)	1.32	27/2852~(0.9%)
3	Q	1.18	3/1585~(0.2%)	1.13	8/2134~(0.4%)
4	R	0.97	3/1571~(0.2%)	1.02	9/2113~(0.4%)
5	S	0.67	0/1420	0.85	0/1907
6	Т	0.67	0/1342	0.83	4/1816~(0.2%)
7	V	0.53	0/1045	0.66	0/1410
8	W	1.10	3/1151~(0.3%)	1.10	7/1551~(0.5%)
9	Х	1.15	0/947	1.20	5/1268~(0.4%)
10	Y	1.30	3/1053~(0.3%)	1.38	12/1403~(0.9%)
11	Ζ	1.13	2/1092~(0.2%)	1.19	6/1460~(0.4%)
12	a	1.27	3/973~(0.3%)	1.30	9/1301~(0.7%)
13	b	0.84	2/901~(0.2%)	1.08	8/1209~(0.7%)
14	с	1.09	3/927~(0.3%)	1.19	7/1240~(0.6%)
15	d	1.32	4/959~(0.4%)	1.37	15/1278~(1.2%)
16	е	1.08	2/828~(0.2%)	1.08	3/1107~(0.3%)
17	f	1.02	1/864~(0.1%)	1.09	1/1156~(0.1%)
18	g	0.91	0/744	1.01	1/994~(0.1%)
19	h	0.82	1/787~(0.1%)	0.89	0/1051
20	i	0.79	0/765	0.87	0/1025
21	j	1.21	2/575~(0.3%)	1.29	7/762~(0.9%)
22	k	1.09	1/634~(0.2%)	1.15	5/848~(0.6%)
23	1	0.71	0/509	1.04	4/677~(0.6%)
24	m	0.87	0/452	1.08	2/605~(0.3%)
25	n	1.16	2/449~(0.4%)	1.42	7/599~(1.2%)
26	0	1.31	7/416~(1.7%)	0.97	1/554~(0.2%)
27	р	1.38	3/379~(0.8%)	1.76	7/498~(1.4%)
28	q	1.15	1/512~(0.2%)	1.26	6/676~(0.9%)
29	r	1.16	1/302~(0.3%)	1.35	5/397~(1.3%)
30	N	1.24	$517/69681~(0.7 \ensuremath{\overline{\%}})$	1.04	$339/108706~(0.3\overline{\%})$
31	L	0.60	0/422	0.78	0/565
32	С	0.28	0/1034	0.52	0/1387



Mol	Chain	B	Bond lengths	I	Bond angles
10101	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
33	U	0.29	0/1122	0.58	0/1515
34	М	0.63	3/1779~(0.2%)	0.83	2/2768~(0.1%)
35	х	0.87	8/1035~(0.8%)	1.12	6/1608~(0.4%)
36	0	0.97	133/36966~(0.4%)	0.93	105/57666~(0.2%)
37	1	0.81	2/1729~(0.1%)	0.93	4/2330~(0.2%)
38	2	0.85	1/1651~(0.1%)	0.95	4/2225~(0.2%)
39	3	0.76	0/1664	0.99	5/2227~(0.2%)
40	4	1.11	1/1118~(0.1%)	1.22	7/1504~(0.5%)
41	5	0.90	1/835~(0.1%)	1.03	3/1128~(0.3%)
42	6	0.66	0/1195	0.95	6/1602~(0.4%)
43	7	0.88	0/988	0.99	2/1326~(0.2%)
44	8	0.86	0/1033	1.13	6/1375~(0.4%)
45	9	0.74	0/796	1.01	3/1077~(0.3%)
46	А	0.86	1/892~(0.1%)	1.03	3/1205~(0.2%)
47	В	1.09	3/968~(0.3%)	1.22	7/1300~(0.5%)
48	D	0.85	1/886~(0.1%)	1.11	9/1186~(0.8%)
49	Ε	0.86	0/784	1.15	7/1043~(0.7%)
50	F	0.94	0/717	1.14	8/959~(0.8%)
51	G	0.94	0/658	1.16	5/884~(0.6%)
52	Н	0.82	0/657	1.02	0/881
53	Ι	0.98	1/462~(0.2%)	1.10	2/621~(0.3%)
54	J	0.81	0/652	1.05	3/877~(0.3%)
55	Κ	0.89	0/670	1.06	3/888~(0.3%)
56	s	1.07	1/430~(0.2%)	1.25	4/570~(0.7%)
57	t	0.34	0/702	0.44	0/973
58	u	0.66	1/1744~(0.1%)	0.86	0/2716
59	V	0.68	3/1282~(0.2%)	0.67	3/1746~(0.2%)
All	All	1.08	$74\overline{7}/162683~(0.5\%)$	1.02	$71\overline{8/243159}~(0.3\%)$

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
2	Р	0	3
3	Q	0	1
5	S	0	2
7	V	0	1
10	Y	0	2
11	Ζ	0	2
19	h	0	1



Mol	Chain	#Chirality outliers	#Planarity outliers
28	q	0	1
30	Ν	0	6
36	0	0	5
37	1	0	2
38	2	0	2
40	4	0	5
41	5	0	2
44	8	0	4
46	А	0	1
47	В	0	2
52	Н	0	2
54	J	0	1
55	Κ	0	1
56	s	0	1
59	V	0	3
All	All	0	50

The worst 5 of 747 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
30	Ν	2873	А	C6-N1	-20.36	1.21	1.35
30	Ν	2765	А	C6-N1	-18.72	1.22	1.35
30	Ν	2502	G	P-OP2	16.57	1.77	1.49
30	Ν	503	А	C6-N1	-15.29	1.24	1.35
30	Ν	1156	А	P-OP2	15.23	1.74	1.49

The worst 5 of 718 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
30	Ν	2506[A]	U	OP1-P-O3'	17.16	142.95	105.20
30	Ν	2506[B]	U	OP1-P-O3'	17.16	142.95	105.20
27	р	39	ARG	NE-CZ-NH1	16.07	128.33	120.30
27	р	39	ARG	NE-CZ-NH2	-14.77	112.92	120.30
34	М	73	С	O3'-P-O5'	14.34	131.24	104.00

There are no chirality outliers.

5 of 50 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	Р	195	VAL	Peptide
2	Р	234	GLY	Peptide



Continued from previous page...

Mol	Chain	Res	Type	Group
2	Р	238	ARG	Peptide
3	Q	151	THR	Peptide
5	S	174	ASP	Peptide

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	ntiles
2	Р	269/273~(98%)	247 (92%)	18 (7%)	4 (2%)	10	45
3	Q	207/209~(99%)	195 (94%)	11 (5%)	1 (0%)	29	69
4	R	199/201~(99%)	191 (96%)	8 (4%)	0	100	100
5	S	175/179~(98%)	163~(93%)	11 (6%)	1 (1%)	25	65
6	Т	174/177~(98%)	165~(95%)	9~(5%)	0	100	100
7	V	139/142~(98%)	112 (81%)	27 (19%)	0	100	100
8	W	140/142~(99%)	136 (97%)	4 (3%)	0	100	100
9	X	120/123~(98%)	109 (91%)	9 (8%)	2(2%)	9	42
10	Y	141/144~(98%)	121 (86%)	16 (11%)	4 (3%)	5	30
11	Z	134/136~(98%)	118 (88%)	11 (8%)	5 (4%)	3	25
12	a	118/127~(93%)	102 (86%)	14 (12%)	2(2%)	9	42
13	b	114/117~(97%)	108 (95%)	6 (5%)	0	100	100
14	с	112/115~(97%)	104 (93%)	8 (7%)	0	100	100
15	d	115/118 (98%)	115 (100%)	0	0	100	100
16	e	101/103~(98%)	92 (91%)	8 (8%)	1 (1%)	15	54
17	f	108/110~(98%)	100 (93%)	7~(6%)	1 (1%)	17	56



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
18	g	91/100~(91%)	80~(88%)	9~(10%)	2(2%)	6	35
19	h	100/104~(96%)	84 (84%)	14 (14%)	2(2%)	7	37
20	i	92/94~(98%)	$89 \ (97\%)$	3(3%)	0	100	100
21	j	73/85~(86%)	71 (97%)	2(3%)	0	100	100
22	k	75/78~(96%)	71 (95%)	3 (4%)	1 (1%)	12	48
23	1	61/63~(97%)	56 (92%)	5 (8%)	0	100	100
24	m	56/59~(95%)	52 (93%)	4 (7%)	0	100	100
25	n	54/57~(95%)	48 (89%)	5 (9%)	1 (2%)	8	38
26	О	48/55~(87%)	45 (94%)	3 (6%)	0	100	100
27	р	44/46~(96%)	40 (91%)	4 (9%)	0	100	100
28	q	62/65~(95%)	56 (90%)	5 (8%)	1 (2%)	9	43
29	r	36/55~(66%)	35 (97%)	1 (3%)	0	100	100
31	L	52/70~(74%)	44 (85%)	7 (14%)	1 (2%)	8	38
32	С	130/223~(58%)	123 (95%)	7 (5%)	0	100	100
33	U	147/149~(99%)	124 (84%)	21 (14%)	2(1%)	11	46
37	1	216/239~(90%)	188 (87%)	27 (12%)	1 (0%)	29	69
38	2	204/218~(94%)	186 (91%)	16 (8%)	2 (1%)	15	54
39	3	203/206~(98%)	182 (90%)	21 (10%)	0	100	100
40	4	148/162 (91%)	116 (78%)	30 (20%)	2(1%)	11	46
41	5	98/131~(75%)	81 (83%)	11 (11%)	6 (6%)	1	16
42	6	149/152~(98%)	139 (93%)	10 (7%)	0	100	100
43	7	127/130~(98%)	121 (95%)	6 (5%)	0	100	100
44	8	125/130~(96%)	103 (82%)	20 (16%)	2(2%)	9	43
45	9	96/103~(93%)	84 (88%)	9 (9%)	3 (3%)	4	27
46	А	115/129~(89%)	102 (89%)	13 (11%)	0	100	100
47	В	121/124 (98%)	104 (86%)	15 (12%)	2(2%)	9	42
48	D	112/118~(95%)	103 (92%)	8 (7%)	1 (1%)	17	56
49	Е	92/101~(91%)	77 (84%)	14 (15%)	1 (1%)	14	51
50	F	86/89~(97%)	81 (94%)	5 (6%)	0	100	100
51	G	80/82~(98%)	69~(86%)	10 (12%)	1 (1%)	12	48
52	Н	78/84~(93%)	66 (85%)	9 (12%)	3 (4%)	3	24



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
53	Ι	53/75~(71%)	49 (92%)	3~(6%)	1 (2%)	8	38
54	J	77/92~(84%)	73~(95%)	4(5%)	0	100	100
55	Κ	83/87~(95%)	78~(94%)	4(5%)	1 (1%)	13	49
56	\mathbf{S}	49/71~(69%)	40 (82%)	9(18%)	0	100	100
57	\mathbf{t}	139/557~(25%)	115~(83%)	21~(15%)	3~(2%)	6	35
59	v	173/182~(95%)	168~(97%)	3~(2%)	2(1%)	13	49
All	All	6111/6981 (88%)	5521 (90%)	528 (9%)	62 (1%)	20	54

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Р	239	ASN
10	Y	36	LYS
11	Ζ	58	LYS
16	е	53	PHE
25	n	55	ILE

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	\mathbf{ntiles}
2	Р	216/218~(99%)	215~(100%)	1 (0%)	88	93
3	Q	164/164~(100%)	161~(98%)	3~(2%)	59	77
4	R	165/165~(100%)	161~(98%)	4 (2%)	49	69
5	S	145/150~(97%)	145~(100%)	0	100	100
6	Т	137/138~(99%)	137~(100%)	0	100	100
7	V	109/110~(99%)	108~(99%)	1 (1%)	78	87
8	W	116/116~(100%)	116 (100%)	0	100	100
9	Х	103/104~(99%)	103~(100%)	0	100	100
10	Y	102/103~(99%)	102 (100%)	0	100	100
11	Z	109/109~(100%)	108 (99%)	1 (1%)	78	87



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
12	a	100/102~(98%)	97~(97%)	3~(3%)	41	63
13	b	86/87~(99%)	86 (100%)	0	100	100
14	с	98/100~(98%)	95~(97%)	3~(3%)	40	62
15	d	89/90~(99%)	88~(99%)	1 (1%)	73	84
16	е	84/84~(100%)	82~(98%)	2(2%)	49	69
17	f	93/93~(100%)	93 (100%)	0	100	100
18	g	80/85~(94%)	80 (100%)	0	100	100
19	h	83/85~(98%)	82 (99%)	1 (1%)	71	83
20	i	78/78~(100%)	78 (100%)	0	100	100
21	j	56/63~(89%)	55 (98%)	1 (2%)	59	77
22	k	67/68~(98%)	67 (100%)	0	100	100
23	1	55/55~(100%)	55 (100%)	0	100	100
24	m	48/49~(98%)	48 (100%)	0	100	100
25	n	47/48~(98%)	46 (98%)	1 (2%)	53	72
26	0	45/49~(92%)	45 (100%)	0	100	100
27	р	38/38~(100%)	38 (100%)	0	100	100
28	q	51/52~(98%)	49 (96%)	2(4%)	32	56
29	r	34/50~(68%)	34 (100%)	0	100	100
31	L	48/63~(76%)	48 (100%)	0	100	100
32	С	110/174~(63%)	110 (100%)	0	100	100
33	U	114/114~(100%)	113 (99%)	1 (1%)	78	87
37	1	179/198~(90%)	177 (99%)	2(1%)	73	84
38	2	170/178~(96%)	169 (99%)	1 (1%)	86	92
39	3	172/173~(99%)	171 (99%)	1 (1%)	86	92
40	4	113/123~(92%)	110 (97%)	3~(3%)	44	65
41	5	87/112 (78%)	86 (99%)	1 (1%)	73	84
42	6	$1\overline{24/125}~(99\%)$	123 (99%)	1 (1%)	81	89
43	7	104/105~(99%)	104 (100%)	0	100	100
44	8	105/107~(98%)	104 (99%)	1 (1%)	76	86
45	9	86/90~(96%)	85 (99%)	1 (1%)	71	83
46	А	$90/\overline{98}~(92\%)$	89 (99%)	1 (1%)	73	84



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
47	В	103/104~(99%)	103 (100%)	0	100	100
48	D	91/96~(95%)	90~(99%)	1 (1%)	73	84
49	Ε	79/83~(95%)	79~(100%)	0	100	100
50	F	75/77~(97%)	74 (99%)	1 (1%)	69	82
51	G	65/65~(100%)	65 (100%)	0	100	100
52	Н	74/77~(96%)	73~(99%)	1 (1%)	67	80
53	Ι	48/66~(73%)	48 (100%)	0	100	100
54	J	70/80~(88%)	68~(97%)	2(3%)	42	64
55	К	65/66~(98%)	65 (100%)	0	100	100
56	S	44/61~(72%)	43 (98%)	1 (2%)	50	70
59	V	108/156~(69%)	108 (100%)	0	100	100
All	All	4922/5244 (94%)	4879 (99%)	43 (1%)	79	87

5 of 43 residues with a non-rotameric side chain are listed below:

Mol	Chain	\mathbf{Res}	Type
39	3	5	LEU
45	9	17	LEU
40	4	15	LEU
41	5	9	MET
48	D	98	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
33	U	28	ASN
41	5	55	HIS
33	U	43	ASN
41	5	3	HIS
44	8	32	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	117/120~(97%)	21 (17%)	1 (0%)
30	Ν	2894/2903~(99%)	521 (18%)	34 (1%)



Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	М	74/75~(98%)	11 (14%)	0
35	Х	43/692~(6%)	34 (79%)	0
36	0	1538/1539~(99%)	280 (18%)	21 (1%)
58	u	72/73~(98%)	19 (26%)	0
All	All	4738/5402 (87%)	886 (18%)	56 (1%)

5 of 886 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	13	G
1	0	25	U
1	0	31	С
1	0	35	С
1	0	41	G

5 of 56 RNA pucker outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
30	Ν	2286	G
36	0	1528	U
36	0	64	G
36	0	1491	G
36	0	1190	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)

Of 3 ligands modelled in this entry, 3 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-13958. 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: 300



Y Index: 300



Z Index: 300



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: 293

Y Index: 289

Z Index: 321

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



6.5 Mask visualisation (i)

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



7 Map analysis (i)

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

7.1 Map-value distribution (i)



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



7.2 Volume estimate (i)



The volume at the recommended contour level is 3383 nm^3 ; this corresponds to an approximate mass of 3056 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 0.175 $\mathrm{\AA^{-1}}$



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-13958 and PDB model 7QGR. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.45 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 Atom inclusion (i)



At the recommended contour level, 54% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

