

wwPDB EM Validation Summary Report (i)

Apr 20, 2024 – 03:26 pm BST

PDB ID	:	7019
EMDB ID	:	EMD-12693
Title	:	Cryo-EM structure of an Escherichia coli TnaC-ribosome complex stalled in
		response to L-tryptophan
Authors	:	van der Stel, A.X.; Gordon, E.R.; Sengupta, A.; Martinez, A.K.; Klepacki, D.;
		Perry, T.N.; Herrero del Valle, A.; Vazquez-Laslop, N.; Sachs, M.S.; Cruz-Vera,
		L.R.; Innis, C.A.
Deposited on	:	2021-03-29
Resolution	:	2.90 Å(reported)
Based on initial model	:	6TBV

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.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	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 chai	in		
1	AA	1534	47%	36%		15% •
2	AB	241	5%		24%	• 7%
3	AC	233	62%		25%	• 12%
4	AD	206	71%		28	3%
5	AE	167	70%		22%	• 7%
6	AF	135	50% 2	7%	·	21%
7	AG	179	59%	2	4% •	16%



Conti	nued fron	n previous	page	
Mol	Chain	Length	Quality of chain	
8	AH	130	65%	34% ••
9	AI	130	• 62%	32% • •
10	AJ	103	5% 51% 43	3% • •
11	AK	129	71%	20% 9%
12	AL	124	80%	19% ••
13	AM	118	57%	40% •
14	AN	102	• 69%	30% •
15	AO	89	78%	21% •
16	AP	82	73%	26% •
17	AQ	84	70%	24% • 5%
18	AR	75	61% 12%	27%
19	AS	92	49% 39%	• 11%
20	AT	87	93%	6% •
21	AU	71	56% 21%	• 21%
22	BA	2897	54% 33%	- 11% •
23	BB	120	66%	27% 6% ·
24	BC	273	83%	15% ••
25	BD	209	88%	11% •
26	BE	201	86%	14%
27	BF	179	78%	20% ••
28	BG	177	79%	20% ••
29	BH	149	70%	30%
30	BI	70	64%	30% 6%
31	BJ	142	86%	13% •
32	BK	123	84%	15% •



Mol	Chain	Length	Quality of chain	
33	BL	144	81%	18% •
34	BM	136	85%	14% •
35	BN	127	83%	10% 7%
36	BO	117	84%	15% •
37	BP	115	86%	11% ••
38	BQ	118	89%	10% •
39	BR	103	83%	17%
40	BS	110	83%	16% •
41	BT	100	78%	15% 7%
42	BU	104	76%	22% •
43	BV	94	72%	27% ·
44	BW	85	78%	12% 11%
45	BX	78	90%	9% •
46	BY	63	86%	13% •
47	BZ	59	83%	15% •
48	B0	57	84%	11% • •
49	B1	55	64%	27% · 7%
50	B2	46	85%	15%
51	B3	65	78%	15% •••
52	B4	38	87%	13%
53	B5	17	82%	12% 6%
54	B7	7	71%	29%
55	B8	77	55% 29%	• 14% •



2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 145019 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 Ribosomal RNA 16S.

Mol	Chain	Residues		I	AltConf	Trace			
1	AA	1534	Total 32930	C 14694	N 6041	O 10661	Р 1534	0	0

• Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	224	Total 1753	C 1109	N 315	0 321	S 8	0	0

• Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	206	Total 1624	C 1028	N 305	0 288	${ m S} { m 3}$	0	0

• Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	205	Total 1643	C 1026	N 315	O 298	${S \atop 4}$	0	0

• Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	155	Total 1144	C 711	N 216	0 211	S 6	0	0

• Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	106	Total 862	C 545	N 156	0 154	S 7	0	0



• Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues		At	oms			AltConf	Trace
7	AG	151	Total 1181	C 735	N 227	0 215	${f S}$ 4	0	0

• Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues		At	oms			AltConf	Trace
8	AH	129	Total 979	C 616	N 173	0 184	S 6	0	0

• Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues		At	oms			AltConf	Trace
9	AI	127	Total 1022	C 634	N 206	0 179	${ m S} { m 3}$	0	0

• Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues		At	oms			AltConf	Trace
10	AJ	99	Total 795	C 498	N 152	0 144	S 1	0	0

• Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues		At	oms			AltConf	Trace
11	AK	117	Total 877	C 540	N 174	0 160	${ m S} { m 3}$	0	0

• Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues		At	\mathbf{oms}			AltConf	Trace
12	AL	123	Total 957	C 591	N 196	0 165	${ m S}{ m 5}$	0	0

• Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues		At	oms			AltConf	Trace
13	AM	114	Total 883	C 546	N 178	0 156	${ m S} { m 3}$	0	0

• Molecule 14 is a protein called 30S ribosomal protein S14.



Mol	Chain	Residues		At	oms			AltConf	Trace
14	AN	101	Total 799	C 498	N 165	O 133	${ m S} { m 3}$	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AN	35	ALA	-	insertion	UNP P0AG59

• Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues		At	oms			AltConf	Trace
15	AO	88	Total 714	C 439	N 144	O 130	S 1	0	0

• Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues		At	oms			AltConf	Trace
16	AP	82	Total 649	C 406	N 128	0 114	S 1	0	0

• Molecule 17 is a protein called 30S ribosomal protein S17.

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

• Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues		Aton	ıs	AltConf	Trace	
18	AR	55	Total 455	C 288	N 86	O 81	0	0

• Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues		At	oms	Atoms					
19	AS	82	Total 656	C 419	N 125	0 110	${ m S} { m 2}$	0	0		

• Molecule 20 is a protein called 30S ribosomal protein S20.



Mol	Chain	Residues		At	oms			AltConf	Trace
20	AT	86	Total 670	C 414	N 138	0 115	${ m S} { m 3}$	0	0

• Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
21	AU	56	Total 465	C 290	N 96	0 78	S 1	0	0

• Molecule 22 is a RNA chain called Ribosomal RNA 23S.

Mol	Chain	Residues			Atoms			AltConf	Trace
22	BA	2897	Total 62209	C 27759	N 11446	O 20107	Р 2897	0	0

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

Mol	Chain	Residues		\mathbf{A}^{\dagger}	AltConf	Trace			
23	BB	120	Total 2569	C 1144	N 468	0 837	Р 120	0	0

• Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues		At	AltConf	Trace			
24	BC	271	Total 2082	C 1288	N 423	0 364	${ m S} 7$	0	0

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

Mol	Chain	Residues		At	oms		AltConf	Trace	
25	BD	209	Total 1566	C 980	N 288	0 294	$\begin{array}{c} \mathrm{S} \\ 4 \end{array}$	0	0

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

Mol	Chain	Residues		At	oms			AltConf	Trace
26	BE	201	Total 1552	C 974	N 283	O 290	${ m S}{ m 5}$	0	0

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



Mol	Chain	Residues		At	oms			AltConf	Trace
27	BF	177	Total 1410	C 899	N 249	O 256	S 6	0	0

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
28	BG	176	Total 1323	C 832	N 243	0 246	${S \over 2}$	0	0

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
29	BH	149	Total 1110	C 699	N 197	0 213	S 1	0	0

• Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
30	BI	66	Total	C	N	0	S	0	0
			522	323	99	94	0		

• Molecule 31 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues		At	AltConf	Trace			
31	BJ	142	Total 1129	С 714	N 212	O 199	$\frac{S}{4}$	0	0

• Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues		At	Atoms					
32	BK	123	Total 946	C 593	N 181	0 166	S 6	0	0	

• Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues		At	oms		AltConf	Trace	
33	BL	144	Total 1053	C 654	N 207	O 190	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 34 is a protein called 50S ribosomal protein L16.



Mol	Chain	Residues		At	oms	AltConf	Trace		
34	BM	136	Total 1075	C 686	N 205	0 178	S 6	0	0

• Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues		At	oms	AltConf	Trace		
35	BN	118	Total 945	C 585	N 194	0 161	${f S}{5}$	0	0

• Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues		At	oms	AltConf	Trace		
36	BO	117	Total 900	C 557	N 179	0 163	S 1	0	0

• Molecule 37 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues		At	oms	AltConf	Trace		
37	BP	114	Total 917	C 574	N 179	0 163	S 1	0	0

• Molecule 38 is a protein called 50S ribosomal protein L20.

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

• Molecule 39 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues		At	AltConf	Trace			
39	BR	103	Total 816	C 516	N 153	0 145	${ m S} { m 2}$	0	0

• Molecule 40 is a protein called 50S ribosomal protein L22.

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

• Molecule 41 is a protein called 50S ribosomal protein L23.



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

• Molecule 42 is a protein called 50S ribosomal protein L24.

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

• Molecule 43 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues		At	oms	AltConf	Trace		
43	BV	94	Total 753	$\begin{array}{c} \mathrm{C} \\ 479 \end{array}$	N 137	0 134	${ m S} { m 3}$	0	0

• Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues		At	\mathbf{oms}		AltConf	Trace	
44	BW	76	Total 580	C 359	N 117	O 103	S 1	0	0

• Molecule 45 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues		At	oms	AltConf	Trace		
45	BX	77	Total 625	C 388	N 129	0 106	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues		Atc	\mathbf{ms}	AltConf	Trace		
46	BV	62	Total	С	Ν	Ο	\mathbf{S}	0	0
40	DI	02	501	308	98	94	1	0	0

• Molecule 47 is a protein called 50S ribosomal protein L30.

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

• Molecule 48 is a protein called 50S ribosomal protein L32.



Mol	Chain	Residues		Atc	\mathbf{ms}			AltConf	Trace
48	B0	56	Total 444	C 269	N 94	O 80	S 1	0	0

• Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues		Aton	ıs	AltConf	Trace	
49	B1	51	Total 414	C 266	N 76	O 72	0	0

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

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
50	B2	46	Total 377	C 228	N 90	O 57	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues		Ate	oms		AltConf	Trace	
51	B3	64	Total 504	C 323	N 105	0 74	${ m S}$ 2	0	0

• Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues		Ato	\mathbf{ms}			AltConf	Trace
52	B4	38	Total 302	C 185	N 65	0 48	$\begin{array}{c} \mathrm{S} \\ 4 \end{array}$	0	0

• Molecule 53 is a protein called Tryptophanase leader peptide.

Mol	Chain	Residues	1	Ator	\mathbf{ns}	AltConf	Trace	
53	B5	17	Total 146	C 94	N 27	O 25	0	0

• Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms			AltConf	Trace		
54	B7	7	Total 146	C 65	N 24	O 50	Р 7	0	0

• Molecule 55 is a RNA chain called P-site tRNA-Pro.



Mol	Chain	Residues	Atoms			AltConf	Trace		
55	B8	77	Total 1646	C 733	N 295	O 541	Р 77	0	0

• Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
56	АА	35	Total Mg 35 35	0
56	ВА	132	Total Mg 132 132	0
56	BC	1	Total Mg 1 1	0
56	BD	1	Total Mg 1 1	0
56	B8	1	Total Mg 1 1	0

• Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
57	AB	1	Total Zn 1 1	0
57	BI	1	Total Zn 1 1	0
57	Β4	1	Total Zn 1 1	0

• Molecule 58 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).





Mol	Chain	Residues	Atoms			AltConf	
58	BA	1	Total	С	N	0	0
			15	11	2	2	

• Molecule 59 is water.

Mol	Chain	Residues	Atoms	AltConf
59	AA	168	Total O 168 168	0
59	AK	1	Total O 1 1	0
59	AM	1	Total O 1 1	0
59	AN	2	Total O 2 2	0
59	ВА	608	Total O 608 608	0
59	BC	7	Total O 7 7	0
59	BD	1	Total O 1 1	0
59	BE	1	Total O 1 1	0
59	BL	2	Total O 2 2	0
59	BN	1	Total O 1 1	0
59	B8	1	Total O 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.

- Chain AA: 47% 36% 15% 386 387 388 389 389 391 392 393 G82 C83 U84 J85
- Molecule 1: Ribosomal RNA 16S







LEU GLY GLY MET ALA ALA ALA CLU GLU GLU CLU CLU PRO ALA ALA GLN PRO LYS GLN GLN GLN GLN GLN GLN CLYS GLY LYS GLY LYS CLY • Molecule 4: 30S ribosomal protein S4 Chain AD: 71% 28% E5. • Molecule 5: 30S ribosomal protein S5 Chain AE: 70% 22% • 7% MET ALA HIS HIS ILE GLU CLV GLV GLN GLN GLN GLY 116 LEU GLY LYS • Molecule 6: 30S ribosomal protein S6 Chain AF: 50% 27% 21% • Molecule 7: 30S ribosomal protein S7 Chain AG: 59% 24% 16%

• Molecule 8: 30S ribosomal protein S8 Chain AH: 65% 34% • Molecule 9: 30S ribosomal protein S9 Chain AI: 62% 32% 23 23 23 털길 124 • Molecule 10: 30S ribosomal protein S10 Chain AJ: 51% 43% • Molecule 11: 30S ribosomal protein S11 Chain AK: 71% 20% MET ALA ALA ALA ALA PRO PRO ILE ARG ARG ARG ARG ARG ARG VAL • Molecule 12: 30S ribosomal protein S12 Chain AL: 80% 19% • Molecule 13: 30S ribosomal protein S13 Chain AM: 57% 40%



V97 N97 R98 898 Q100 Q100 R101 102 R101 102 R101 110 R113 R113 R113 R113 R115 R113 R115 R15 R115 R15 R15 R15

 \bullet Molecule 14: 30S ribosomal protein S14



 \bullet Molecule 18: 30S ribosomal protein S18



• Molecule 19: 30S ribosomal protein S19





6% •

ALA ASP LYS LYS ALA LYS LYS LYS

• Molecule 20: 30S ribosomal protein S20

Chain AT:



 \bullet Molecule 21: 30S ribosomal protein S21

Chain AU: 56% 21% 21% 21%

93%

 \bullet Molecule 22: Ribosomal RNA 23S









 \bullet Molecule 26: 50S ribosomal protein L4







 \bullet Molecule 28: 50S ribosomal protein L6



G161 V162 A165 A165 R170 K177

• Molecule 29: 50S ribosomal protein L9





 \bullet Molecule 31: 50S ribosomal protein L13



Chain BJ:	86%	13% •
M1 P8 D19 T21 C22 C22	A23 L36 L36 P46 P46 P46 P46 F411 F114 F113 F113 F113 F114 F113 F113	
• Molecule	32: 50S ribosomal protein L14	
Chain BK:	84%	15% •
M1 138 139 143 143	P46 D56 D56 D56 D56 D56 D56 D56 D57 P12 P122 P120 P120 P120 P120 P120 P122 P122	
• Molecule	33: 50S ribosomal protein L15	
Chain BL:	81%	18% •
M1 P8 812 K13	L13 C13 C13 C13 C13 C13 C13 C13 C	
• Molecule	34: 50S ribosomal protein L16	
Chain BM:	85%	14% •
M1 P4 L20	F11 V36 R44 R44 R55 R55 R55 P169 P17 P109 F110 F129 F110 F129 F125 F129 F129 F129 F129 F129	
• Molecule	35: 50S ribosomal protein L17	
Chain BN:	83%	10% 7%
M1 M20 M24 B32 B32	K35 P50 P50 P50 P50 P50 P50 P50 P50 P50 P5	
• Molecule	36: 50S ribosomal protein L18	
Chain BO:	84%	15% •
M1 R16 E20 V27	F3 2 140 141 141 142 143 143 144 143 144 143 144 143 144 143 144 143 144 143 144 143 144 143 144 144	
• Molecule	37: 50S ribosomal protein L19	
Chain BP:	86%	11% ••
MET 82 E9 P18 P22	W31 E34 E34 K38 R33 R53 E68 F33 F33 R33 F33 F33 F112 E114 E112 E114 E112 E114	

 \bullet Molecule 38: 50S ribosomal protein L20



Chain BQ:	89%	10% •
MET A2 A3 K5 K6 A35 A35	A118 A118 A118 A118 A118 A118	
• Molecule 3	9: 50S ribosomal protein L21	
Chain BR:	83%	17%
M1 Q6 K10 Q11 R13 R13	E22 E22 141 141 644 644 644 646 650 050 050 051 751 853 853 853 853 853 853 853 853 853 853	
• Molecule 4	0: 50S ribosomal protein L22	
Chain BS:	83%	16% ·
M E2 R11 K48 E52 E52	L33 166 172 172 172 173 173 173 173 173 173 173 173 173 173	
• Molecule 4	1: 50S ribosomal protein L23	
Chain BT:	78%	15% 7%
M1 12 E4 E5 E1 L11 P14	E18 1722 1722 1722 1722 1722 1722 1722 17	
• Molecule 4	2: 50S ribosomal protein L24	
Chain BU:	76%	22% •
MET A2 R7 D8 D18 V18	N22 N22 V28 V28 N24 N25 N46 N46 N46 N53 N53 N55 N46 N53 N55 N55 N55 N55 N55 N55 N55 N55 N55	
• Molecule 4	3: 50S ribosomal protein L25	
Chain BV:	72%	27% •
M1 F2 E7 K10 K14	M24 M24 M25 F26 F26 F26 F26 F26 F26 F26 F26 F26 F26	A 94
• Molecule 4	4: 50S ribosomal protein L27	
Chain BW:	78%	12% 11%
MET ALA ALA LYS LYS LYS ALA GLY SER SER	A18 K19 F26 F26 F26 F29 F41 F74 F74 F78 F78 F78 F78	

 \bullet Molecule 45: 50S ribosomal protein L28



Chain BX:	90%		9% •
MET S2 P12 P12 P12 P12 E43 R44 R44 R44 R45 R45 R45 R45 R45			
• Molecule 46: 50S ribe	osomal protein L29		
Chain BY:	86%		13% ·
MET K2 K3 K4 K4 E5 E5 C4 C4 C4 C4 C4 C4 C4 C4 C4 C4 C4 C4 C4	R R R R R R R R R R R R R R R R R R R		
• Molecule 47: 50S ribo	osomal protein L30		
Chain BZ:	83%	1	.5% •
MET A2 74 74 74 74 83 837 74 853 759 148 148 148 148 148 148 148 159			
• Molecule 48: 50S ribo	osomal protein L32		
Chain B0:	84%	1:	۱% ۰۰
MET A2 P8 D31 C32 C32 C32 C32 C43 C43 C44 D46 D46 D46			
• Molecule 49: 50S ribe	osomal protein L33		
Chain B1:	64%	27%	• 7%
MET ALA LLYS LYS LYS 15 16 19 19 19 12 12 12 12 12 12 12 21 12 21 12 21 12 21 12 21 12 21 12 21 12 12	P31 K37 K37 K37 P41 V42 V43 R44 K46 K50 E51 I54 I54 LYS		
• Molecule 50: 50S ribo	osomal protein L34		
Chain B2:	85%		15%
M1 14 14 12 12 12 12 12 12 12 12 12 12 12 12 12			
• Molecule 51: 50S ribo	osomal protein L35		
Chain B3:	78%	15%	•••
MET P2 K12 K12 K12 M28 M26 H26 H26 H26 H26 H28 L33 L33 L33 L33 K36 K36 K36	P 46 K 44 A 48 P 63 A 65 A 65		
• Molecule 52: 50S ribo	osomal protein L36		



Chain B4:	87%	13%
M1 116 V26 A29 E30 P31		
• Molecule 5	3: Tryptophanase leader peptide	
Chain B5:	82%	12% 6%
V8 N14 R23 P24		
• Molecule 54	4: mRNA	
Chain B7:	71%	29%
c1 c2 c3 c3 c5 c5 c5 c5 c5 c5 c5 c5		
• Molecule 5	5: P-site tRNA-Pro	
Chain B8:	55% 29%	14% •
C1 62 63 65 65 A1 4 1 4	U17 U17 018 018 020 022 022 022 022 022 022 022 022 02	671 672 672 674 476 476



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	93588	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{\AA}^2)$	40	Depositor
Minimum defocus (nm)	-1000	Depositor
Maximum defocus (nm)	-2000	Depositor
Magnification	55127	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.094	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0075	Depositor
Map size (Å)	370.056, 370.056, 370.056	wwPDB
Map dimensions	408, 408, 408	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.907, 0.907, 0.907	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, UR3, 4OC, ZN, 6MZ, 4D4, OMU, 3TD, 5MC, OMC, 2MG, MA6, D2T, 1MG, MEQ, OMG, 2MA, 5MU, PSU, G7M

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		Bond lengths		Bond angles		
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	AA	1.49	1045/36593~(2.9%)	3.42	4438/57081~(7.8%)	
2	AB	0.81	7/1784~(0.4%)	0.57	1/2403~(0.0%)	
3	AC	0.83	7/1651~(0.4%)	0.51	0/2225	
4	AD	0.78	6/1665~(0.4%)	0.47	0/2227	
5	AE	0.87	5/1157~(0.4%)	0.57	0/1557	
6	AF	1.05	7/881~(0.8%)	0.59	0/1189	
7	AG	0.93	7/1195~(0.6%)	0.51	0/1602	
8	AH	0.90	5/989~(0.5%)	0.55	0/1326	
9	AI	0.73	3/1034~(0.3%)	0.66	3/1375~(0.2%)	
10	AJ	1.03	6/805~(0.7%)	0.56	0/1089	
11	AK	1.09	7/893~(0.8%)	0.57	0/1205	
12	AL	1.12	8/960~(0.8%)	0.59	1/1286~(0.1%)	
13	AM	0.93	5/892~(0.6%)	0.61	0/1193	
14	AN	0.88	4/811~(0.5%)	0.53	0/1081	
15	AO	0.36	0/722	0.47	0/964	
16	AP	0.76	2/659~(0.3%)	0.54	0/884	
17	AQ	0.76	2/657~(0.3%)	0.57	0/881	
18	AR	0.87	2/462~(0.4%)	0.54	0/621	
19	AS	1.08	5/672~(0.7%)	0.59	0/904	
20	AT	0.54	1/676~(0.1%)	0.43	0/895	
21	AU	1.08	4/472~(0.8%)	0.56	1/627~(0.2%)	
22	BA	1.84	1753/69120~(2.5%)	3.52	8456/107824~(7.8%)	
23	BB	1.53	58/2872~(2.0%)	3.02	271/4478~(6.1%)	
24	BC	1.20	19/2121~(0.9%)	0.66	0/2852	
25	BD	0.95	7/1576~(0.4%)	0.59	0/2119	
26	BE	0.85	5/1571~(0.3%)	0.57	0/2113	
27	BF	0.85	6/1434~(0.4%)	0.52	0/1926	
28	BG	1.00	8/1343~(0.6%)	0.58	0/1816	
29	BH	0.70	3/1121~(0.3%)	0.56	0/1515	
30	BI	0.80	2/531~(0.4%)	0.60	0/709	
31	BJ	1.03	6/1152~(0.5%)	0.56	0/1551	



Mal	Chain	I	Bond lengths		Bond angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
32	BK	1.00	5/955~(0.5%)	0.67	1/1279~(0.1%)
33	BL	0.90	4/1062~(0.4%)	0.64	1/1413~(0.1%)
34	BM	1.09	7/1081~(0.6%)	0.59	0/1443
35	BN	0.98	4/958~(0.4%)	0.59	0/1281
36	BO	0.74	2/910~(0.2%)	0.54	0/1219
37	BP	0.90	3/929~(0.3%)	0.64	2/1242~(0.2%)
38	BQ	0.72	0/960	0.49	0/1278
39	BR	0.81	2/829~(0.2%)	0.56	0/1107
40	BS	0.76	2/864~(0.2%)	0.53	0/1156
41	BT	0.67	1/744~(0.1%)	0.56	0/994
42	BU	0.89	3/787~(0.4%)	0.58	0/1051
43	BV	1.01	4/766~(0.5%)	0.58	0/1025
44	BW	0.80	1/587~(0.2%)	0.57	0/776
45	BX	0.87	2/635~(0.3%)	0.59	0/848
46	BY	0.43	0/502	0.46	0/667
47	ΒZ	0.91	2/453~(0.4%)	0.57	0/605
48	B0	0.82	1/450~(0.2%)	0.64	1/599~(0.2%)
49	B1	1.19	5/421~(1.2%)	0.76	2/561~(0.4%)
50	B2	0.85	1/380~(0.3%)	0.60	0/498
51	B3	1.12	4/513~(0.8%)	0.74	1/676~(0.1%)
52	B4	0.88	1/303~(0.3%)	0.54	0/397
53	B5	1.51	2/150~(1.3%)	0.71	0/203
54	B7	0.31	0/161	1.06	0/248
55	B8	1.94	66/1839~(3.6%)	2.95	$15\overline{2/2866}~(5.3\%)$
All	All	1.54	3127/155710~(2.0%)	3.00	$1333\overline{1/232950}~(5.7\%)$

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
10	AJ	0	1
27	BF	0	1
51	B3	0	1
All	All	0	3

The worst 5 of 3127 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
22	BA	892	А	C2'-C1'	-21.93	1.29	1.53
22	BA	2449	U	C5-C6	20.02	1.52	1.34



Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
55	B8	14	A	C6-N6	17.45	1.48	1.33
55	B8	59	А	C6-N6	17.43	1.47	1.33
55	B8	76	A	C6-N6	17.33	1.47	1.33

The worst 5 of 13331 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
22	BA	2451	A	N1-C6-N6	-24.52	103.89	118.60
22	BA	2872	А	N1-C6-N6	-23.89	104.27	118.60
22	BA	1668	A	N1-C6-N6	-23.68	104.39	118.60
22	BA	1668	А	C2-N3-C4	23.56	122.38	110.60
22	BA	1668	А	N1-C2-N3	-23.30	117.65	129.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	AJ	81	GLU	Peptide
51	B3	31	HIS	Peptide
27	BF	142	ASP	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	AA	32930	0	16591	430	0
2	AB	1753	0	1780	43	0
3	AC	1624	0	1696	36	0
4	AD	1643	0	1707	41	0
5	AE	1144	0	1185	26	0
6	AF	862	0	864	28	0
7	AG	1181	0	1238	35	0
8	AH	979	0	1031	32	0
9	AI	1022	0	1070	45	0
10	AJ	795	0	836	35	0
11	AK	877	0	887	24	0
12	AL	957	0	1017	14	0



Conti	nuea fron	<i>i</i> previous	page			
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	AM	883	0	941	50	0
14	AN	799	0	841	26	0
15	AO	714	0	734	13	0
16	AP	649	0	666	16	0
17	AQ	648	0	691	13	0
18	AR	455	0	478	7	0
19	AS	656	0	680	34	0
20	AT	670	0	719	3	0
21	AU	465	0	491	17	0
22	BA	62209	0	31308	391	0
23	BB	2569	0	1301	15	0
24	BC	2082	0	2154	19	0
25	BD	1566	0	1618	15	0
26	BE	1552	0	1619	15	0
27	BF	1410	0	1444	30	0
28	BG	1323	0	1371	18	0
29	BH	1110	0	1148	32	0
30	BI	522	0	520	20	0
31	BJ	1129	0	1162	11	0
32	BK	946	0	1023	12	0
33	BL	1053	0	1129	18	0
34	BM	1075	0	1155	9	0
35	BN	945	0	989	8	0
36	BO	900	0	935	11	0
37	BP	917	0	962	12	0
38	BQ	947	0	1019	12	0
39	BR	816	0	839	11	0
40	BS	857	0	922	11	0
41	BT	738	0	807	12	0
42	BU	779	0	831	15	0
43	BV	753	0	780	15	0
44	BW	580	0	594	6	0
45	BX	625	0	652	4	0
46	BY	501	0	531	5	0
47	BZ	449	0	488	4	0
48	B0	444	0	458	5	0
49	B1	414	0	442	11	0
50	B2	377	0	418	7	0
51	B3	504	0	572	11	0
52	B4	302	0	340	3	0
53	B5	146	0	143	2	0
54	B7	146	0	77	4	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	B8	1646	0	831	19	0
56	AA	35	0	0	0	0
56	B8	1	0	0	0	0
56	BA	132	0	0	1	0
56	BC	1	0	0	0	0
56	BD	1	0	0	0	0
57	AB	1	0	0	0	0
57	B4	1	0	0	0	0
57	BI	1	0	0	0	0
58	BA	15	0	9	0	0
59	AA	168	0	0	3	0
59	AK	1	0	0	0	0
59	AM	1	0	0	0	0
59	AN	2	0	0	0	0
59	B8	1	0	0	1	0
59	BA	608	0	0	4	0
59	BC	7	0	0	0	0
59	BD	1	0	0	0	0
59	BE	1	0	0	0	0
59	BL	2	0	0	0	0
59	BN	1	0	0	0	0
All	All	145019	0	96734	1531	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 1531 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)
22:BA:962:G:OP1	59:BA:3201:HOH:O	1.58	1.19
22:BA:2107:G:H1	22:BA:2182:U:H3	1.03	1.01
22:BA:2133:G:N2	22:BA:2158:A:N6	2.12	0.98
13:AM:53:ILE:HG22	13:AM:57:ARG:HH21	1.26	0.97
22:BA:2133:G:N2	22:BA:2158:A:C6	2.35	0.94

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
2	AB	222/241~(92%)	209 (94%)	13~(6%)	0	100	100
3	AC	204/233~(88%)	198 (97%)	6 (3%)	0	100	100
4	AD	203/206~(98%)	196 (97%)	7 (3%)	0	100	100
5	AE	153/167~(92%)	148 (97%)	5(3%)	0	100	100
6	AF	104/135~(77%)	102 (98%)	2(2%)	0	100	100
7	AG	149/179~(83%)	143~(96%)	6 (4%)	0	100	100
8	AH	127/130~(98%)	127 (100%)	0	0	100	100
9	AI	125/130~(96%)	115 (92%)	10 (8%)	0	100	100
10	AJ	97/103~(94%)	89 (92%)	6 (6%)	2(2%)	7	26
11	AK	115/129~(89%)	111 (96%)	4 (4%)	0	100	100
12	AL	120/124~(97%)	113 (94%)	7 (6%)	0	100	100
13	AM	112/118~(95%)	104 (93%)	8 (7%)	0	100	100
14	AN	99/102~(97%)	88 (89%)	11 (11%)	0	100	100
15	AO	86/89~(97%)	82~(95%)	4(5%)	0	100	100
16	AP	80/82~(98%)	73 (91%)	7 (9%)	0	100	100
17	AQ	78/84~(93%)	76~(97%)	2(3%)	0	100	100
18	AR	53/75~(71%)	52 (98%)	1 (2%)	0	100	100
19	AS	80/92~(87%)	74 (92%)	6 (8%)	0	100	100
20	AT	84/87~(97%)	84 (100%)	0	0	100	100
21	AU	54/71~(76%)	52 (96%)	2(4%)	0	100	100
24	BC	269/273~(98%)	260 (97%)	9(3%)	0	100	100
25	BD	206/209~(99%)	198 (96%)	7 (3%)	1 (0%)	29	61
26	BE	$199/201 \ (99\%)$	192 (96%)	7 (4%)	0	100	100
27	BF	175/179~(98%)	171 (98%)	4 (2%)	0	100	100
28	BG	174/177~(98%)	173 (99%)	1 (1%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
29	BH	147/149~(99%)	133 (90%)	14 (10%)	0	100	100
30	BI	64/70~(91%)	58 (91%)	6 (9%)	0	100	100
31	BJ	140/142~(99%)	140 (100%)	0	0	100	100
32	BK	121/123~(98%)	119 (98%)	2(2%)	0	100	100
33	BL	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
34	BM	133/136~(98%)	130 (98%)	3 (2%)	0	100	100
35	BN	116/127~(91%)	109 (94%)	7 (6%)	0	100	100
36	BO	115/117~(98%)	113 (98%)	2 (2%)	0	100	100
37	BP	112/115~(97%)	109 (97%)	3 (3%)	0	100	100
38	BQ	115/118 (98%)	115 (100%)	0	0	100	100
39	BR	101/103~(98%)	98~(97%)	3 (3%)	0	100	100
40	BS	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
41	BT	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
42	BU	100/104 (96%)	96 (96%)	4 (4%)	0	100	100
43	BV	92/94~(98%)	91 (99%)	1 (1%)	0	100	100
44	BW	74/85~(87%)	73~(99%)	1 (1%)	0	100	100
45	BX	75/78~(96%)	72 (96%)	3 (4%)	0	100	100
46	BY	60/63~(95%)	59 (98%)	1 (2%)	0	100	100
47	BZ	56/59~(95%)	55 (98%)	1 (2%)	0	100	100
48	B0	54/57~(95%)	53 (98%)	1 (2%)	0	100	100
49	B1	49/55~(89%)	48 (98%)	1 (2%)	0	100	100
50	B2	44/46~(96%)	41 (93%)	3 (7%)	0	100	100
51	B3	62/65~(95%)	57 (92%)	3 (5%)	2 (3%)	4	16
52	B4	36/38~(95%)	36 (100%)	0	0	100	100
53	B5	15/17~(88%)	14 (93%)	1 (7%)	0	100	100
All	All	5590/5931~(94%)	5378 (96%)	207 (4%)	5 (0%)	54	82

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	BD	149	ASN
51	B3	32	ILE
51	B3	33	LEU



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Mol	Chain	Res	Type
10	AJ	57	VAL
10	AJ	58	ASN

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	ntiles
2	AB	186/199~(94%)	183~(98%)	3~(2%)	62	86
3	AC	170/190~(90%)	168~(99%)	2(1%)	71	91
4	AD	172/173~(99%)	172 (100%)	0	100	100
5	AE	118/126~(94%)	118 (100%)	0	100	100
6	AF	92/116~(79%)	92 (100%)	0	100	100
7	AG	124/147~(84%)	123 (99%)	1 (1%)	81	94
8	AH	104/105~(99%)	104 (100%)	0	100	100
9	AI	105/107~(98%)	104 (99%)	1 (1%)	76	92
10	AJ	87/90~(97%)	87 (100%)	0	100	100
11	AK	90/99~(91%)	90 (100%)	0	100	100
12	AL	102/103~(99%)	102 (100%)	0	100	100
13	AM	92/96~(96%)	92 (100%)	0	100	100
14	AN	79/84~(94%)	78~(99%)	1 (1%)	69	90
15	AO	76/77~(99%)	76 (100%)	0	100	100
16	AP	65/65~(100%)	65 (100%)	0	100	100
17	AQ	74/78~(95%)	74 (100%)	0	100	100
18	AR	48/65~(74%)	48 (100%)	0	100	100
19	AS	71/79~(90%)	70~(99%)	1 (1%)	67	89
20	AT	65/66~(98%)	65 (100%)	0	100	100
21	AU	48/61~(79%)	48 (100%)	0	100	100
24	BC	216/218~(99%)	216 (100%)	0	100	100
25	BD	163/163~(100%)	162 (99%)	1 (1%)	86	96



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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	BE	165/165~(100%)	165~(100%)	0	100	100
27	$_{\mathrm{BF}}$	148/150~(99%)	147~(99%)	1 (1%)	84	95
28	BG	137/138~(99%)	136 (99%)	1 (1%)	84	95
29	BH	114/114 (100%)	114 (100%)	0	100	100
30	BI	59/62~(95%)	58~(98%)	1 (2%)	60	86
31	BJ	116/116~(100%)	116 (100%)	0	100	100
32	BK	104/104 (100%)	103 (99%)	1 (1%)	76	92
33	BL	103/103~(100%)	103 (100%)	0	100	100
34	BM	108/108~(100%)	108 (100%)	0	100	100
35	BN	98/103~(95%)	98 (100%)	0	100	100
36	BO	87/87~(100%)	86~(99%)	1 (1%)	73	92
37	BP	99/100~(99%)	99 (100%)	0	100	100
38	BQ	89/90~(99%)	89 (100%)	0	100	100
39	BR	84/84~(100%)	84 (100%)	0	100	100
40	BS	93/93~(100%)	93~(100%)	0	100	100
41	BT	80/84~(95%)	80 (100%)	0	100	100
42	BU	83/85~(98%)	83 (100%)	0	100	100
43	BV	78/78~(100%)	78 (100%)	0	100	100
44	BW	57/63~(90%)	57~(100%)	0	100	100
45	BX	67/68~(98%)	67~(100%)	0	100	100
46	BY	54/55~(98%)	54 (100%)	0	100	100
47	BZ	48/49~(98%)	48 (100%)	0	100	100
48	B0	47/48~(98%)	46 (98%)	1 (2%)	53	81
49	B1	45/49~(92%)	45 (100%)	0	100	100
50	B2	38/38 (100%)	38 (100%)	0	100	100
51	B3	51/52~(98%)	51 (100%)	0	100	100
52	B4	34/34~(100%)	34 (100%)	0	100	100
53	B5	17/17~(100%)	16 (94%)	1 (6%)	19	49
All	All	4650/4844 (96%)	4633 (100%)	17 (0%)	91	97

 $5~{\rm of}~17$ residues with a non-rotameric side chain are listed below:



Mol	Chain	Res	Type
36	BO	63	LYS
53	B5	24	PRO
14	AN	27	LYS
19	AS	29	LYS
25	BD	33	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
53	B5	17	ASN
53	B5	14	ASN
28	BG	38	ASN
8	AH	18	GLN
36	BO	43	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1530/1534~(99%)	238~(15%)	7(0%)
22	BA	2890/2897~(99%)	417 (14%)	23~(0%)
23	BB	119/120~(99%)	13 (10%)	1 (0%)
54	B7	6/7~(85%)	3~(50%)	1(16%)
55	B8	76/77~(98%)	12~(15%)	2(2%)
All	All	4621/4635~(99%)	683~(14%)	34~(0%)

5 of 683 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	7	А
1	AA	9	G
1	AA	22	G
1	AA	32	А

5 of 34 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	BA	2518	А
22	BA	2873	А
55	B8	2	G
22	BA	984	А



Continued from previous page...

\mathbf{Mol}	Chain	\mathbf{Res}	Type
22	BA	784	G

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

37 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Turne	Chain	Ros Link		Bond lengths		B	ond ang	les	
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
22	1MG	BA	745	22	18,26,27	2.36	5 (27%)	19,39,42	1.44	2 (10%)
22	G7M	BA	2069	22	20,26,27	2.14	6 (30%)	17,39,42	1.25	2 (11%)
22	PSU	BA	2580	22	18,21,22	3.77	7 (38%)	22,30,33	2.14	6 (27%)
1	5MC	AA	1407	1	18,22,23	3.26	7 (38%)	26,32,35	1.00	1 (3%)
22	OMG	BA	2251	22,55	18,26,27	2.30	8 (44%)	19,38,41	1.86	4 (21%)
1	MA6	AA	1518	1	18,26,27	1.34	2 (11%)	19,38,41	3.38	2 (10%)
22	PSU	BA	1911	22	18,21,22	4.12	6 (33%)	22,30,33	2.00	5 (22%)
22	2MG	BA	2445	22	18,26,27	2.28	6 (33%)	16,38,41	1.80	4 (25%)
22	PSU	BA	746	22,56	18,21,22	1.47	3 (16%)	22,30,33	2.42	5 (22%)
22	5MU	BA	1939	22	19,22,23	0.76	0	28,32,35	1.17	3 (10%)
25	MEQ	BD	150	25	8,9,10	1.37	2 (25%)	5,10,12	1.46	1 (20%)
1	UR3	AA	1498	1	19,22,23	3.03	8 (42%)	26,32,35	1.40	3 (11%)
1	2MG	AA	1207	1	18,26,27	2.45	7 (38%)	16,38,41	1.42	4 (25%)
1	4OC	AA	1402	1	20,23,24	2.90	8 (40%)	26,32,35	0.97	2 (7%)
22	5MU	BA	747	22	19,22,23	0.82	1 (5%)	28,32,35	1.26	3 (10%)
22	6MZ	BA	1618	22	18,25,26	2.93	5 (27%)	16,36,39	2.21	4 (25%)
22	6MZ	BA	2030	22	18,25,26	2.95	5 (27%)	16,36,39	2.58	4 (25%)
22	PSU	BA	955	22	18,21,22	3.80	6 (33%)	22,30,33	2.17	5 (22%)
22	2MA	BA	2503	22,56	17,25,26	2.30	5 (29%)	17,37,40	1.43	4 (23%)
1	5MC	AA	967	1	18,22,23	3.43	7 (38%)	26,32,35	1.06	2 (7%)
22	5MC	BA	1962	22	18,22,23	3.07	7 (38%)	26,32,35	1.26	5 (19%)
1	MA6	AA	1519	1	18,26,27	1.32	1 (5%)	19,38,41	3.57	2 (10%)



Mol	Type	Chain	Bos	Link	Bo	ond leng	ths	B	ond ang	gles
WIOI	Type	Ullalli	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
22	OMC	BA	2498	22,56	19,22,23	2.64	7 (36%)	26,31,34	1.05	1 (3%)
1	2MG	AA	1516	1	18,26,27	2.32	7 (38%)	16,38,41	1.48	4 (25%)
22	3TD	BA	1915	22	18,22,23	4.06	8 (44%)	22,32,35	1.97	4 (18%)
1	2MG	AA	966	1	18,26,27	2.46	7 (38%)	16,38,41	1.46	3 (18%)
34	4D4	BM	81	34	9,11,12	2.44	3 (33%)	8,13,15	1.06	0
22	2MG	BA	1835	22	18,26,27	2.19	7 (38%)	16,38,41	1.70	4 (25%)
22	PSU	BA	1917	22	18,21,22	4.07	7 (38%)	22,30,33	1.88	5 (22%)
22	PSU	BA	2605	22	18,21,22	<mark>3.73</mark>	7 (38%)	22,30,33	1.88	4 (18%)
12	D2T	AL	89	12	7,9,10	1.07	0	6,11,13	2.56	2 (33%)
22	OMU	BA	2552	22	19,22,23	2.64	7 (36%)	26,31,34	1.92	5 (19%)
1	G7M	AA	527	1	20,26,27	2.43	6 (30%)	17,39,42	1.09	1 (5%)
22	PSU	BA	2504	22	18,21,22	3.88	6 (33%)	22,30,33	1.72	4 (18%)
22	PSU	BA	2457	22	18,21,22	<mark>3.66</mark>	7 (38%)	22,30,33	2.28	5 (22%)
1	PSU	AA	516	56,1	18,21,22	4.19	6 (33%)	22,30,33	1.95	6 (27%)
22	PSU	BA	2604	22	18,21,22	3.82	6 (33%)	22,30,33	2.05	5 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	1MG	BA	745	22	-	0/3/25/26	0/3/3/3
22	G7M	BA	2069	22	-	1/3/25/26	0/3/3/3
22	PSU	BA	2580	22	-	1/7/25/26	0/2/2/2
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
22	OMG	BA	2251	$22,\!55$	-	3/5/27/28	0/3/3/3
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
22	PSU	BA	1911	22	-	2/7/25/26	0/2/2/2
22	$2 \mathrm{MG}$	BA	2445	22	-	2/5/27/28	0/3/3/3
22	PSU	BA	746	$22,\!56$	-	2/7/25/26	0/2/2/2
22	5MU	BA	1939	22	-	2/7/25/26	0/2/2/2
25	MEQ	BD	150	25	-	2/8/9/11	-
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
1	2MG	AA	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	AA	1402	1	-	$1\overline{/9/29/30}$	0/2/2/2
22	5MU	BA	747	$2\overline{2}$	_	$0/7/\overline{25}/26$	0/2/2/2
22	6MZ	BA	1618	22	-	$0\overline{/5/27/28}$	0/3/3/3



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	6MZ	BA	2030	22	-	2/5/27/28	0/3/3/3
22	PSU	BA	955	22	-	0/7/25/26	0/2/2/2
22	2MA	BA	2503	22,56	-	1/3/25/26	0/3/3/3
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
22	5MC	BA	1962	22	-	0/7/25/26	0/2/2/2
1	MA6	AA	1519	1	-	2/7/29/30	0/3/3/3
22	OMC	BA	2498	22,56	-	2/9/27/28	0/2/2/2
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
22	3TD	BA	1915	22	-	2/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	2/5/27/28	0/3/3/3
34	4D4	BM	81	34	-	2/11/12/14	-
22	2MG	BA	1835	22	-	0/5/27/28	0/3/3/3
22	PSU	BA	1917	22	-	0/7/25/26	0/2/2/2
22	PSU	BA	2605	22	-	0/7/25/26	0/2/2/2
12	D2T	AL	89	12	-	1/7/12/14	-
22	OMU	BA	2552	22	-	0/9/27/28	0/2/2/2
1	G7M	AA	527	1	-	2/3/25/26	0/3/3/3
22	PSU	BA	2504	22	-	2/7/25/26	0/2/2/2
22	PSU	BA	2457	22	-	0/7/25/26	0/2/2/2
1	PSU	AA	516	56,1	-	0/7/25/26	0/2/2/2
22	PSU	BA	2604	22	-	0/7/25/26	0/2/2/2

The worst 5 of 203 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1915	3TD	C6-C5	11.67	1.48	1.35
1	AA	516	PSU	C6-C5	11.19	1.48	1.35
22	BA	1911	PSU	C6-C5	10.95	1.48	1.35
22	BA	1618	6MZ	C6-N6	10.93	1.52	1.35
22	BA	2030	6MZ	C6-N6	10.86	1.52	1.35

The worst 5 of 126 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	AA	1519	MA6	N1-C6-N6	-13.95	102.37	117.06
1	AA	1518	MA6	N1-C6-N6	-13.36	103.00	117.06
22	BA	746	PSU	N1-C2-N3	7.79	123.96	115.13
22	BA	1915	3TD	N1-C2-N3	6.40	121.19	116.14
1	AA	1519	MA6	N3-C2-N1	-6.28	118.86	128.68



There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
1	AA	527	G7M	C3'-C4'-C5'-O5'
1	AA	966	2MG	O4'-C4'-C5'-O5'
34	BM	81	4D4	NE-CD-CG-CB
22	BA	746	PSU	C2'-C1'-C5-C4
22	BA	1915	3TD	C3'-C4'-C5'-O5'

5 of 34 torsion outliers are listed below:

There are no ring outliers.

12 mon	omers ar	e involv	ved in 13	short cont	acts:
Mol	Chain	Res	Type	Clashes	Symm

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	BA	2251	OMG	1	0
1	AA	1518	MA6	1	0
22	BA	746	PSU	1	0
25	BD	150	MEQ	1	0
1	AA	1402	4OC	1	0
22	BA	2030	6MZ	3	0
22	BA	955	PSU	1	0
1	AA	1519	MA6	1	0
22	BA	2498	OMC	1	0
1	AA	1516	2MG	1	0
12	AL	89	D2T	1	0
1	AA	527	G7M	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 174 ligands modelled in this entry, 173 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mol	Tuno	Chain	Chain	Chain	Chain	Dog	Link	Bond lengths			B	ond ang	les
	Type		nes	LIUK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2			
58	TRP	BA	3001	-	14,16,16	0.86	1 (7%)	16,22,22	1.13	2 (12%)			

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	TRP	BA	3001	-	-	0/7/8/8	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(Å)	Ideal(Å)
58	BA	3001	TRP	OXT-C	-2.20	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
58	BA	3001	TRP	OXT-C-O	-2.59	118.21	124.09
58	BA	3001	TRP	OXT-C-CA	2.15	120.71	113.38

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	BA	2

All chain breaks are listed below:



Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	885:C	O3'	892:A	Р	13.83
1	BA	2099:U	O3'	2100:G	Р	3.52



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-12693. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



6.1.2 Raw map



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



6.2 Central slices (i)

6.2.1 Primary map



X Index: 204





Z Index: 204

6.2.2 Raw map



X Index: 204

Y Index: 204



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: 219





Z Index: 188

6.3.2 Raw map



X Index: 219

Y Index: 196



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



6.4.2 Raw 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 0.0075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.



6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.6.1 emd_12693_msk_1.map (i)



I



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 3192 nm^3 ; this corresponds to an approximate mass of 2883 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 0.345 \AA^{-1}



8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.345 $\mathrm{\AA^{-1}}$



8.2 Resolution estimates (i)

$\begin{bmatrix} Bosolution ostimato (Å) \end{bmatrix}$	Estimation criterion (FSC cut-off)		
Resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.87	3.18	2.90
Unmasked-calculated*	3.17	4.33	3.22

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-12693 and PDB model 7O19. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.0075 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 (0.0075).



9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	$\mathbf{Q} extsf{-score}$
All	0.9870	0.5550
AA	0.9920	0.5160
AB	0.8310	0.4000
AC	0.9560	0.4400
AD	0.9540	0.4560
AE	0.9950	0.5140
AF	0.9680	0.4860
AG	0.9600	0.4210
AH	0.9840	0.5180
AI	0.9600	0.4200
AJ	0.8910	0.3800
AK	0.9930	0.5200
AL	0.9970	0.5400
AM	0.9690	0.4510
AN	0.9810	0.4340
AO	0.9870	0.5240
AP	0.9940	0.5160
AQ	0.9980	0.5170
AR	1.0000	0.5170
AS	0.9610	0.4170
AT	0.9800	0.5330
AU	0.9120	0.4360
B0	0.9930	0.6040
B1	1.0000	0.5900
B2	1.0000	0.6400
B3	1.0000	0.6290
B4	1.0000	0.6250
B5	1.0000	0.4990
B7	1.0000	0.4410
B8	0.9990	0.4470
BA	0.9950	0.5930
BB	0.9980	0.5930
BC	1.0000	0.6240
BD	0.9930	0.6170
BE	0.9780	0.5860

0.0 <0.0

1.0



Chain	Atom inclusion	Q-score
BF	0.9910	0.5010
BG	0.9760	0.5380
BH	0.8620	0.4080
BI	0.8560	0.3820
BJ	0.9950	0.6200
BK	0.9990	0.6120
BL	0.9850	0.6040
BM	0.9930	0.6100
BN	1.0000	0.6330
BO	0.9840	0.5800
BP	0.9980	0.6020
BQ	0.9980	0.6300
BR	0.9600	0.5950
BS	0.9890	0.6120
BT	0.9900	0.5810
BU	0.9880	0.5730
BV	0.9730	0.5840
BW	0.9860	0.6090
BX	0.9980	0.6040
BY	0.9860	0.5660
BZ	0.9770	0.5990

