

wwPDB EM Validation Summary Report (i)

Apr 27, 2024 – 01:20 PM EDT

PDB ID	:	8UU8
EMDB ID	:	EMD-42571
Title	:	Cryo-EM structure of the Listeria innocua 70S ribosome (head-swiveled) in
		complex with HflXr and pe/E-tRNA (structure II-C)
Authors	:	Seely, S.M.; Basu, R.S.; Gagnon, M.G.
Deposited on	:	2023-10-31
Resolution	:	3.10 Å(reported)
Based on initial model	:	7NHN

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	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

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



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$		
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	a	1550	76%	22% •
2	b	249	83%	• 16%
3	с	218	39%	6%
4	d	200	• 100%	
5	е	167	• 91%	9%
6	f	97	97%	
7	g	156	83%	17%
8	h	132	99%	



Conti	nued fron	n previous	page	
Mol	Chain	Length	Quality of chain	
9	i	130	28%	·
10	j	102	93%	• 6%
11	k	129	88%	12%
12	1	137	96%	••
13	m	121	54% 89%	11%
14	n	61	82%	18%
15	О	89	98%	•
16	р	90	• 96%	••
17	q	87	92%	8%
18	r	79	81%	19%
19	s	92	68%	20%
20	t	84	96%	•
21	х	76	67% 28%	• •
22	W	21	24% 14% 29% 57%	
23	v	418	9%	
24	А	2932	. 83%	16% ·
25	В	116	88%	10% •
26	С	277	99%	·
27	D	209	99%	·
28	Е	207	99%	•
29	F	179	97%	••
30	G	178	96%	•
31	Ι	166	78%	22%
	тт	1/1	6U%	
32	П	141	94%	• •



Mol	Chain	Length	Quality of chain	
34	М	122	100%	
35	Ν	146	100%	
36	0	144	94%	6%
37	Р	135	90%	10%
38	Q	119	8%	
39	R	114	99%	
40	S	119	99%	
41	Т	102	99%	
42	U	118	95%	5%
43	V	94	97%	•••
44	W	103	99%	
45	Y	96	79%	21%
46	Ζ	62	95%	5%
47	1	63	95%	5%
48	2	59	95%	5%
49	3	81	88%	• 10%
50	4	57	93%	7%
51	5	49	98%	·
52	6	44	98%	
53	7	66	97%	·
54	8	37	97%	•



2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 142031 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 16S Ribosomal RNA.

Mol	Chain	Residues		1	AltConf	Trace			
1	a	1516	Total 32515	C 14504	N 5960	O 10535	Р 1516	0	0

• Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	209	Total 1396	C 888	N 249	O 255	S 4	0	0

• Molecule 3 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
3	с	204	Total 1003	C 595	N 204	O 204	0	0

• Molecule 4 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues		At	oms	AltConf	Trace		
4	d	199	Total 1562	C 978	N 289	O 293	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 5 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	е	152	Total 1057	C 666	N 197	0 192	${S \over 2}$	0	0

• Molecule 6 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	95	Total 785	C 496	N 138	0 149	${S \over 2}$	0	0



• Molecule 7 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues		At	\mathbf{oms}			AltConf	Trace
7	g	130	Total 650	C 387	N 130	0 132	S 1	0	0

• Molecule 8 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues		At	oms	AltConf	Trace		
8	h	131	Total 1022	C 651	N 180	0 189	${ m S} { m 2}$	0	0

• Molecule 9 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace	
9	i	127	Total 635	C 377	N 128	O 130	0	0

• Molecule 10 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues		Aton	ns	AltConf	Trace	
10	j	96	Total 477	C 285	N 96	O 96	0	0

• Molecule 11 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues		At	oms	AltConf	Trace		
11	k	114	Total 748	C 455	N 149	0 141	${ m S} { m 3}$	0	0

• Molecule 12 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues		At	oms	AltConf	Trace		
12	1	135	Total 993	C 615	N 198	0 179	S 1	0	0

• Molecule 13 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
13	m	108	Total 529	C 313	N 108	O 108	0	0

• Molecule 14 is a protein called Small ribosomal subunit protein uS14.



Mol	Chain	Residues		Atc	\mathbf{ms}	AltConf	Trace		
14	n	50	Total 260	C 154	N 53	O 50	${ m S} { m 3}$	0	0

• Molecule 15 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues		At	oms	AltConf	Trace		
15	О	87	Total 695	C 431	N 137	0 125	${ m S} { m 2}$	0	0

• Molecule 16 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues		At	oms	AltConf	Trace		
16	р	88	Total 661	C 418	N 126	0 114	${ m S} { m 3}$	0	0

• Molecule 17 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues		At	oms	AltConf	Trace		
17	q	80	Total 650	C 410	N 120	O 119	S 1	0	0

• Molecule 18 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
18	r	64	Total	С	Ν	Ο	S	0	0
10	1	04	494	319	93	81	1	0	0

• Molecule 19 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues		Aton	ıs	AltConf	Trace	
19	S	74	Total 365	C 217	N 74	О 74	0	0

• Molecule 20 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues		At	oms			AltConf	Trace
20	t	81	Total 583	C 353	N 117	0 112	S 1	0	0

 $\bullet\,$ Molecule 21 is a RNA chain called pe/E Hybrid State Phenylalanine tRNA.



Mol	Chain	Residues		-	Atom	s			AltConf	Trace
21	x	74	Total 1591	C 713	N 285	O 517	Р 74	${ m S} { m 2}$	0	0

• Molecule 22 is a RNA chain called F-Stop mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	9	Total 190	C 86	N 34	O 61	Р 9	0	0

• Molecule 23 is a protein called GTPase HflX.

Mol	Chain	Residues		At	oms			AltConf	Trace
23	V	417	Total 3282	C 2067	N 566	O 639	S 10	0	0

• Molecule 24 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues			Atoms			AltConf	Trace
24	А	2901	Total 62318	C 27812	N 11528	O 20077	Р 2901	0	0

• Molecule 25 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues		A	AltConf	Trace			
25	В	114	Total 2428	C 1082	N 428	0 804	Р 114	0	0

• Molecule 26 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues		At		AltConf	Trace		
26	С	274	Total 2084	C 1293	N 408	O 376	S 7	0	0

• Molecule 27 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues		At	oms			AltConf	Trace
27	D	206	Total 1544	C 975	N 288	0 277	${f S}$ 4	0	0

• Molecule 28 is a protein called Large ribosomal subunit protein uL4.



Mol	Chain	Residues		Ato	ms		AltConf	Trace
28	Е	205	Total 1536	C 976	N 286	0 274	0	0

• Molecule 29 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues		At	oms	AltConf	Trace		
29	F	175	Total 1173	C 732	N 215	0 222	$\frac{S}{4}$	0	0

• Molecule 30 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues		At	oms	AltConf	Trace		
30	G	171	Total 1305	C 822	N 241	0 241	S 1	0	0

• Molecule 31 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
31	Ι	129	Total 636	C 378	N 129	O 129	0	0

• Molecule 32 is a protein called Large ribosomal subunit protein uL11.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
32	Н	135	Total 673	C 403	N 135	O 135	0	0

• Molecule 33 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues		At	oms	AltConf	Trace		
33	L	143	Total 1112	C 707	N 205	0 197	${ m S} { m 3}$	0	0

• Molecule 34 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues		At	AltConf	Trace			
34	М	122	Total 893	C 554	N 170	0 165	${S \atop 4}$	0	0

• Molecule 35 is a protein called Large ribosomal subunit protein uL15.



Mol	Chain	Residues		At	AltConf	Trace			
35	N	146	Total 1071	C 662	N 209	O 199	S 1	0	0

• Molecule 36 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues		At	AltConf	Trace			
36	О	135	Total 1062	C 679	N 203	0 174	S 6	0	0

• Molecule 37 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues		At	AltConf	Trace			
37	Р	122	Total 982	C 616	N 193	0 172	S 1	0	0

• Molecule 38 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues		At	AltConf	Trace			
38	Q	119	Total 884	C 545	N 172	O 166	S 1	0	0

• Molecule 39 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues		At	oms	AltConf	Trace		
39	R	113	Total 885	C 560	N 171	0 153	S 1	0	0

• Molecule 40 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues		At	AltConf	Trace			
40	S	118	Total 949	C 602	N 187	O 156	${f S}$ 4	0	0

• Molecule 41 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues		At	AltConf	Trace			
41	Т	101	Total 774	C 502	N 134	0 137	S 1	0	0

• Molecule 42 is a protein called Large ribosomal subunit protein uL22.



Mol	Chain	Residues		Ato	ms		AltConf	Trace
42	U	112	Total 850	$\begin{array}{c} \mathrm{C} \\ 537 \end{array}$	N 159	O 154	0	0

• Molecule 43 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues		At	oms	AltConf	Trace		
43	V	92	Total 726	C 463	N 126	0 134	${ m S} { m 3}$	0	0

• Molecule 44 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues		At	oms			AltConf	Trace
44	W	102	Total 760	C 482	N 140	0 135	${ m S} { m 3}$	0	0

• Molecule 45 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues		At	oms			AltConf	Trace
45	Y	76	Total 567	C 347	N 110	O 109	S 1	0	0

• Molecule 46 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues		Ato	\mathbf{ms}			AltConf	Trace
46	Z	59	Total 444	С 274	N 92	O 76	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 47 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues		Atc	\mathbf{ms}			AltConf	Trace
47	1	60	Total	С	Ν	Ο	S	0	0
47	L	00	477	295	94	87	1	0	0

• Molecule 48 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues		Atc	\mathbf{ms}			AltConf	Trace
48	2	56	Total 433	C 272	N 82	0 78	S 1	0	0

• Molecule 49 is a protein called Large ribosomal subunit protein bL31B.



Mol	Chain	Residues		At	oms			AltConf	Trace
49	3	73	Total 523	C 328	N 90	O 104	S 1	0	0

• Molecule 50 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
50	4	53	Total	C	N 86	0 70	S E	0	0
			417	230	80	70	Э		

• Molecule 51 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
51	5	48	Total 394	C 241	N 79	O 70	$\frac{S}{4}$	0	0

• Molecule 52 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues		Atc	\mathbf{ms}			AltConf	Trace
50	6	12	Total	С	Ν	Ο	S	0	0
52	0	40	365	222	88	53	2	0	0

• Molecule 53 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
53	7	64	Total 520	C 322	N 114	O 79	${f S}{5}$	0	0

• Molecule 54 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues		Ato	\mathbf{ms}			AltConf	Trace
54	8	36	Total 280	C 174	N 56	0 44	S 6	0	0

• Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
55	a	151	Total Mg 151 151	0
55	b	1	Total Mg 1 1	0
55	с	1	Total Mg 1 1	0



Mol	Chain	Residues	Atoms	AltConf
55	g	1	Total Mg 1 1	0
55	i	2	Total Mg 2 2	0
55	m	1	Total Mg 1 1	0
55	n	2	Total Mg 2 2	0
55	0	1	Total Mg 1 1	0
55	V	2	Total Mg 2 2	0
55	А	249	Total Mg 249 249	0
55	В	5	Total Mg 5 5	0
55	С	1	Total Mg 1 1	0
55	D	2	Total Mg 2 2	0
55	М	1	Total Mg 1 1	0
55	Ν	1	Total Mg 1 1	0
55	S	1	Total Mg 1 1	0
55	W	1	Total Mg 1 1	0

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• Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
56	n	1	Total Zn 1 1	0
56	4	1	Total Zn 1 1	0
56	5	1	Total Zn 1 1	0
56	8	1	Total Zn 1 1	0

• Molecule 57 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).





Mol	Chain	Residues	Atoms			AltConf		
57	V	1	Total	С	Ν	Ο	Р	0
	1	32	11	5	13	3	0	

• Molecule 58 is water.

Mol	Chain	Residues	Atoms	AltConf
58	a	94	Total O 94 94	0
58	d	1	Total O 1 1	0
58	е	1	Total O 1 1	0
58	f	1	Total O 1 1	0
58	i	1	Total O 1 1	0
58	р	3	Total O 3 3	0
58	t	1	Total O 1 1	0
58	V	2	Total O 2 2	0
58	А	235	Total O 235 235	0
58	В	6	Total O 6 6	0
58	С	2	Total O 2 2	0



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Mol	Chain	Residues	Atoms	AltConf
58	D	1	Total O 1 1	0
58	Ν	5	Total O 5 5	0
58	О	1	Total O 1 1	0
58	Р	1	Total O 1 1	0
58	S	2	Total O 2 2	0
58	Т	1	Total O 1 1	0
58	U	2	Total O 2 2	0
58	V	1	Total O 1 1	0
58	Z	2	Total O 2 2	0
58	2	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.

• Molecule 1: 16S Ribosomal RNA











 \bullet Molecule 3: Small ribosomal subunit protein uS3





• Molecule 6: Small ribosomal subunit protein bS6

GLU GLU GLU GLU

MET PRO GLU GLU ILE ASP GLY ASN ASN LEU LEU











• Molecule 18: Small ribosomal subunit protein bS18

Chain r:	81%	19%	-
MET ALA GLY GLY GLY GLY GLY ARG ARG ARG ARG ARG ARG CLY C	LYSS CLUB		
• Molecule 19: Small	ribosomal subunit protein uS1	19	
Chain s:	68% 80%	20%	-
MET GLY R3 R3 R4 K7 K7 C8 C8 C9 C9 F10 V11 D12 D13	H14 L15 M16 M16 M17 M17 K19 M21 M21 M21 M22 M22 M22 M22 M22 M22 M22	132 133 133 133 135 135 135 133 143 143 143 143	F44 V45 Q46 Q47 Q47 T48 T48 K56 K56 K56 K56 K56 K56 K56 K56 K56 K56
D65 M66 V67 V67 C68 H69 K70 C72 E73 F74 F74 F75	ARG THR TTR ARG GLY HIS ALA ASP ASP ASP ASP LYS THR THR THR THR ARG		
• Molecule 20: Small	ribosomal subunit protein bS2	20	
Chain t:	96%		-
MET P2 N41 044 LNS LNS			
• Molecule 21: pe/E	Hybrid State Phenylalanine tF	RNA	
Chain x:	87% 67%	28% •	·
61 63 63 65 47 48 49 65 49 61 0 110 611	414 615 615 619 619 622 622 625 626 626 626 626 620 620 620 620 620 630	Call Control C	044 045 046 046 048 048 058 053 053 053 053 053 053 055 055 055 055
C61 C62 C62 A64 A64 A64 C65 C65 C66 C66 C68 C72 C72	A73 C74 A76 A76		
• Molecule 22: F-Stop	o mRNA		
Chain w: 14%	29%	57%	_
C C C C C C C C C C C C C C C C C C C			
• Molecule 23: GTPa	se HflX		
Chain v:	100%		-
	W O R L D W I PROTEIN DATA	BANK	



• Molecule 24: 23S Ribosomal RNA





C2207 C2210 C2211 C2211 C2214 C2211 C2215 C2215 C2215 C2216 C2218 C2218 C2218 C2218 C2218 C2218 C2218 C2218 C2218 C2216 C2226 C2216 C2226 C2226 C2226 C2216 C2226 C226
C2380 C2381 A2391 A2394 A2394 A2394 C2418 C2418 C2418 C2418 C2418 C2418 C2418 C2418 C2418 C2438 C2448 A2463 C2474 A2463 C2474 A2463 C2475 C2476 A2668 U2568 U2568 U2568 C2643 C2643 C2668 C2668 C2668 C2643 C2668 C2643 C2668 C2643 C2643 C2643 C2643 C2643
U2646 V2647 V2648 V2648 V2648 C2679 C2679 C2694 C2679 C2694 C2679 C2694 C2695 C2755 C2756 V2759 C2756 C2852 C28555 C28555 C28555 C28555 C28555 C28555 C28555 C28555
 Molecule 25: 5S Ribosomal RNA
Chain B: 88% 10% .
U U U U U U U U U U U U U U
• Molecule 26: Large ribosomal subunit protein uL2
Chain C: 99%
MET A2 H2 14 H2 15 H2 15 H
• Molecule 27: Large ribosomal subunit protein uL3
Chain D: 99%
MET T2 ALA LYS
• Molecule 28: Large ribosomal subunit protein uL4
Chain E: 99% ·
MET P2 P2 ALA
• Molecule 29: Large ribosomal subunit protein uL5
Chain F: 97% ···





V132 R133 E134 Q135 L136 P139	V143 P144 P144 V146 V146 V148 R150 E164 E164 E165 E165 C174 M175 P176 P176 P176 P176 P176 P176 P176 P177 P177			
• Molecule 30:	Large ribosomal subunit protein uL6			
Chain G:	96%			
MET SER ARG ILE G5 K6 A13 C14	N20 621 52 836 846 846 8117 8117 8117 8119 8119 8119 8119 8119			
• Molecule 31:	Large ribosomal subunit protein uL10			
Chain I:	78%	22%		
M1 S2 K3 V4 A7 S10 S10	V12 E13 E14 F15 F15 F17 F17 F16 F15 F15 F15 F125 F22 F22 F22 F22 F22 F22 F22 F22 F22 F	V35 636 636 138 139 140 141 145 145 145	D47 A48 A48 E51 F52 K53 K53 V54	N5 S58 L59 R61 R62 A63
V64 E85 A66 N67 G68 C68 F70 C71	E73 674 A75 L76 L76 A81 A81 A81 A83 B81 A83 B85 B87 B85 B87 B86 A91 B87 B87 B87 B87 B87 B87 B87 B87 B87 B87	L96 N97 P98 F99 A100 K101 D102 H103 E104 A105 E104	1108 K109 A110 C111 V112 E114 E114 C115 C115	V117 V117 A118 S119 E120 E121 E122 E122 K124
A125 L126 A127 T128 L129 P120 P120 P120 ARG CLU GLU	LEU LEU SER MET LEU CYS CYS CYS CYS CYS CLEU CLEU CLEU CLEU CLU CYS CLU CYS CLU	GLU GLU ALA		
• Molecule 32:	Large ribosomal subunit protein uL11			
Chain H:	94%	• •		
MET LALA LALA LALS K3 K7 K7 E8 E8	L11 L11 L11 L11 L11 L11 L11 L11 L11 A15 A15 A16 A15 A15 A15 A15 A16 A17 A27 A31 A33 A33 A34 A34 A44 A44	T46 A47 A47 A50 A50 A50 F51 F53 F55 F55 V56	V57 F61 E62 E62 864 S65 F66 T70	K71 172 173 ₩73
L78 L79 K80 K81 A82 A83 K84 V88 V88 V88 E86	K87 P32 N35 K94 N35 K94 N36 N36 N396 N496 N496 N400 C101 C101 C101 C102 C105 C115 C105 C115 C105 C115 C105 C115 C105 C115 C105 C115 C105 C115 C105 C115	P114 D115 L116 A119 A119 V121 V121 E122 S123 A124 A124 M126	V128	
• Molecule 33:	Large ribosomal subunit protein uL13			

Chain L:

99%



• Molecule 34: Large ribosomal subunit protein uL14



.

Chain M:	100%	
There are no outlier residues reco	orded for this chain.	
• Molecule 35: Large ribosomal s	subunit protein uL15	
Chain N:	100%	
M1 1146		
• Molecule 36: Large ribosomal s	subunit protein uL16	
Chain O:	94%	6%
M1 E135 CLUU CLUU CLUY CLUY CLUY CLUY CLUY CLUY		
• Molecule 37: Large ribosomal s	subunit protein bL17	
Chain P:	90%	10%
MET GLY 73 73 75 76 776 476 476 417 1176 417 617 517 717 717 717 717 717 717 717 717 7		
• Molecule 38: Large ribosomal s	subunit protein uL18	
Chain Q:	100%	
M1 12 13 14 15 16 16 865 865 865 865 865 865 865 8116		
• Molecule 39: Large ribosomal s	subunit protein bL19	
Chain R:	99%	
MI D16 G35 A113 A113 A113		
• Molecule 40: Large ribosomal s	subunit protein bL20	
Chain S:	99%	
MET P2 K119		
• Molecule 41: Large ribosomal s	subunit protein bL21	



Chain T:	99%	
M1 B44 N101 ALA		
• Molecule 42: Large riboso	mal subunit protein uL22	
Chain U:	95%	5%
ALA SER ES VII5 CUU GUV GUV		
• Molecule 43: Large riboso	mal subunit protein uL23	
Chain V:	97%	
M1 F91 GLU GLU VAL		
• Molecule 44: Large riboso	mal subunit protein uL24	
Chain W:	99%	.
M1 150 152 952 952 973 873 873 873 873 885 687 886 886 888 888	TYS	
• Molecule 45: Large riboso	mal subunit protein bL27	
Chain Y:	79%	21%
MET LEU LYS LYS ALA ALA ALA ALA ALA ALA CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY	ALA ALA	
• Molecule 46: Large riboso	mal subunit protein bL28	
Chain Z:	95%	5%
MET A2 E60 ARG VAL		
• Molecule 47: Large riboso	mal subunit protein uL29	
Chain 1:	95%	5%
MET LYS A3 ALA ALA		
• Molecule 48: Large riboso	mal subunit protein uL30	



Chain 2:	95%	5%	
MET ALA K3 E58 VAL			
• Molecule 49: Large r	ibosomal subunit protein bL31B		
Chain 3:	65% 88%	• 10%	
MI 64 79 79 712 717 717	S18 T19 F21 F22 F23 F23 F24 F25 S25 S25 S25 S25 S25 S31 S32 S31 S31 S32 S31 S32 S31 S32 S31 S32 S31 S32 S31 S32 S33 S34 S35 S36 S31 S32 S33 S34 S35 S35 S36 S37 S38 S31 S32 S33 S34 S35 S35 S36 S37 S38 S38 S39 S40 S41 S41 S42 S44 S44 S44 S44 S44 S44 S44 S44 <	L45 R47 R47 R47 F48 E49 S51 S51 S52 S53 H55 F55 F55 F55 F55 F55 F55 F55 F55 F55	GLN LYS HIS ALA
THR AG7 D68 C699 R70 077 P71 F74 F74 K77 Y78 Y78			
• Molecule 50: Large r	ibosomal subunit protein bL32		
Chain 4:	93%	7%	
MET A2 K52 D53 D53 ASN ASN SER			
• Molecule 51: Large r	ibosomal subunit protein bL33		
Chain 5:	98%		
M1 E25 T48 LYS			
• Molecule 52: Large r	ibosomal subunit protein bL34		
Chain 6:	98%		
<mark>И 1</mark> 843 Ага			
• Molecule 53: Large r	ibosomal subunit protein bL35		
Chain 7:	97%		
MET P2 M65 LYS			
• Molecule 54: Large r	ibosomal subunit protein bL36		
Chain 8:	97%		







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	55099	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	40.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	34.334	Depositor
Minimum map value	-17.982	Depositor
Average map value	0.002	Depositor
Map value standard deviation	1.124	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	435.2, 435.2, 435.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	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: 4SU, GCP, MG, PSU, ZN, MIA, 5MU, 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).

Mal	Chain	Bond	lengths	E	Bond angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	a	0.54	0/36403	0.88	12/56778~(0.0%)
2	b	0.29	0/1419	0.55	1/1945~(0.1%)
3	с	0.24	0/1002	0.45	0/1391
4	d	0.32	0/1590	0.56	0/2142
5	е	0.34	0/1069	0.55	0/1451
6	f	0.32	0/797	0.60	0/1068
7	g	0.24	0/649	0.41	0/901
8	h	0.37	0/1035	0.61	0/1392
9	i	0.27	0/636	0.49	0/878
10	j	0.24	0/476	0.48	0/663
11	k	0.27	0/760	0.53	0/1031
12	l	0.33	0/1009	0.61	1/1365~(0.1%)
13	m	0.24	0/528	0.45	0/731
14	n	0.27	0/259	0.56	0/357
15	0	0.33	0/705	0.63	0/949
16	р	0.33	0/674	0.59	0/909
17	q	0.32	0/659	0.57	0/882
18	r	0.34	0/502	0.60	0/673
19	s	0.24	0/364	0.45	0/505
20	\mathbf{t}	0.29	0/586	0.55	0/788
21	Х	0.26	0/1605	0.82	0/2497
22	W	0.29	0/212	0.81	0/327
23	V	0.30	0/3324	0.54	0/4483
24	А	0.51	0/69819	0.79	3/108917~(0.0%)
25	В	0.32	0/2711	0.75	0/4224
26	С	0.32	0/2120	0.54	0/2848
27	D	0.35	0/1566	0.55	0/2108
28	Ε	0.31	0/1557	0.52	0/2103
29	F	0.26	0/1186	0.56	0/1615
30	G	0.28	0/1327	0.52	0/1793
31	Ι	0.23	0/635	0.40	0/882
32	Н	0.26	0/676	0.42	0/942



Mal	Chain	Bond	lengths	E	Bond angles
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5
33	L	0.33	0/1135	0.50	0/1526
34	М	0.33	0/900	0.56	0/1212
35	N	0.31	0/1082	0.54	0/1446
36	0	0.32	0/1084	0.55	0/1450
37	Р	0.32	0/993	0.57	0/1328
38	Q	0.26	0/893	0.54	0/1201
39	R	0.32	0/897	0.57	0/1206
40	S	0.34	0/962	0.50	0/1280
41	Т	0.37	0/787	0.50	0/1057
42	U	0.32	0/860	0.54	0/1165
43	V	0.32	0/735	0.51	0/988
44	W	0.30	0/770	0.50	0/1032
45	Y	0.33	0/574	0.58	0/766
46	Z	0.30	0/449	0.56	0/597
47	1	0.26	0/478	0.52	0/640
48	2	0.28	0/436	0.53	0/585
49	3	0.26	0/532	0.49	0/720
50	4	0.36	0/425	0.58	0/567
51	5	0.30	0/398	0.58	0/534
52	6	0.33	0/368	0.64	0/479
53	7	0.31	0/527	0.62	0/685
54	8	0.32	0/283	0.53	0/375
All	All	0.47	0/153428	0.76	$17/230377 \ (0.0\%)$

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
12	1	0	1
16	р	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	b	130	PRO	CA-N-CD	-7.68	100.75	111.50
1	а	1012	G	O4'-C1'-N9	6.58	113.47	108.20
1	a	1260	G	C6-C5-N7	-6.52	126.49	130.40
1	a	1017	С	C2-N1-C1'	6.21	125.63	118.80



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	а	1260	G	N3-C4-N9	6.14	129.69	126.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	1	57	LYS	Peptide
16	р	45	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	entiles
2	b	207/249~(83%)	180 (87%)	26 (13%)	1 (0%)	29	64
3	с	202/218~(93%)	176 (87%)	26 (13%)	0	100	100
4	d	197/200~(98%)	181 (92%)	16 (8%)	0	100	100
5	е	150/167~(90%)	137 (91%)	13 (9%)	0	100	100
6	f	93/97~(96%)	72 (77%)	20 (22%)	1 (1%)	14	46
7	g	128/156~(82%)	118 (92%)	10 (8%)	0	100	100
8	h	129/132~(98%)	115 (89%)	14 (11%)	0	100	100
9	i	125/130~(96%)	105 (84%)	20 (16%)	0	100	100
10	j	94/102~(92%)	71 (76%)	22 (23%)	1 (1%)	14	46
11	k	112/129~(87%)	100 (89%)	12 (11%)	0	100	100
12	1	133/137~(97%)	120 (90%)	13 (10%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
13	m	106/121~(88%)	92~(87%)	14 (13%)	0	100	100
14	n	48/61~(79%)	33~(69%)	15 (31%)	0	100	100
15	О	85/89~(96%)	78~(92%)	7 (8%)	0	100	100
16	р	86/90~(96%)	74 (86%)	11 (13%)	1 (1%)	13	44
17	q	78/87~(90%)	71 (91%)	7 (9%)	0	100	100
18	r	62/79~(78%)	56 (90%)	6 (10%)	0	100	100
19	s	72/92~(78%)	65~(90%)	7 (10%)	0	100	100
20	t	79/84~(94%)	77 (98%)	2 (2%)	0	100	100
23	V	415/418 (99%)	382 (92%)	33 (8%)	0	100	100
26	С	272/277~(98%)	261 (96%)	10 (4%)	1 (0%)	34	69
27	D	204/209~(98%)	194 (95%)	10 (5%)	0	100	100
28	Ε	203/207~(98%)	189 (93%)	14 (7%)	0	100	100
29	F	173/179~(97%)	161 (93%)	12 (7%)	0	100	100
30	G	169/178~(95%)	156 (92%)	13 (8%)	0	100	100
31	Ι	127/166~(76%)	122 (96%)	5 (4%)	0	100	100
32	Н	133/141~(94%)	122 (92%)	9 (7%)	2(2%)	10	39
33	L	141/145~(97%)	135~(96%)	6 (4%)	0	100	100
34	М	120/122~(98%)	115~(96%)	5 (4%)	0	100	100
35	Ν	144/146~(99%)	133 (92%)	11 (8%)	0	100	100
36	Ο	133/144~(92%)	129~(97%)	4 (3%)	0	100	100
37	Р	118/135~(87%)	113 (96%)	5 (4%)	0	100	100
38	Q	117/119~(98%)	107 (92%)	10 (8%)	0	100	100
39	R	111/114~(97%)	104 (94%)	7 (6%)	0	100	100
40	S	116/119~(98%)	113 (97%)	3(3%)	0	100	100
41	Т	99/102~(97%)	96~(97%)	3(3%)	0	100	100
42	U	110/118~(93%)	107 (97%)	3(3%)	0	100	100
43	V	$90/\overline{94}~(96\%)$	84 (93%)	5 (6%)	1 (1%)	14	46
44	W	100/103~(97%)	98~(98%)	2(2%)	0	100	100
45	Y	74/96~(77%)	68 (92%)	6 (8%)	0	100	100
46	Z	57/62~(92%)	53 (93%)	4 (7%)	0	100	100
47	1	58/63~(92%)	56 (97%)	2 (3%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentile	s
48	2	54/59~(92%)	51 (94%)	3~(6%)	0	100 100	
49	3	69/81~(85%)	61 (88%)	7 (10%)	1 (1%)	11 40	
50	4	51/57~(90%)	44 (86%)	7 (14%)	0	100 100	
51	5	46/49~(94%)	45~(98%)	1 (2%)	0	100 100	
52	6	41/44~(93%)	41 (100%)	0	0	100 100	
53	7	62/66~(94%)	57 (92%)	5 (8%)	0	100 100	
54	8	34/37~(92%)	32 (94%)	2(6%)	0	100 100	
All	All	5827/6270~(93%)	5350 (92%)	468 (8%)	9~(0%)	50 79	

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	j	79	PRO
16	р	25	SER
32	Н	92	PRO
49	3	56	PRO
2	b	129	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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
2	b	104/214~(49%)	104 (100%)	0	100	100
4	d	162/170~(95%)	162 (100%)	0	100	100
5	е	104/131~(79%)	104 (100%)	0	100	100
6	f	81/85~(95%)	81 (100%)	0	100	100
7	g	4/130~(3%)	4 (100%)	0	100	100
8	h	109/110~(99%)	109 (100%)	0	100	100
9	i	4/102~(4%)	4 (100%)	0	100	100
11	k	58/100~(58%)	58 (100%)	0	100	100
12	1	101/118~(86%)	100 (99%)	1 (1%)	76	90



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	n	5/52~(10%)	5~(100%)	0	100	100
15	О	71/81~(88%)	71 (100%)	0	100	100
16	р	63/80~(79%)	63 (100%)	0	100	100
17	q	72/78~(92%)	72 (100%)	0	100	100
18	r	47/67~(70%)	47 (100%)	0	100	100
20	t	55/66~(83%)	55 (100%)	0	100	100
23	v	351/365~(96%)	351 (100%)	0	100	100
26	С	215/225~(96%)	215 (100%)	0	100	100
27	D	158/171~(92%)	158 (100%)	0	100	100
28	Е	161/174~(92%)	161 (100%)	0	100	100
29	F	93/155~(60%)	91 (98%)	2 (2%)	52	78
30	G	139/147~(95%)	139 (100%)	0	100	100
32	Н	4/111 (4%)	4 (100%)	0	100	100
33	L	116/121~(96%)	116 (100%)	0	100	100
34	М	92/101 (91%)	92 (100%)	0	100	100
35	Ν	105/115~(91%)	105 (100%)	0	100	100
36	О	105/113~(93%)	105 (100%)	0	100	100
37	Р	102/111~(92%)	102 (100%)	0	100	100
38	Q	88/97~(91%)	88 (100%)	0	100	100
39	R	93/99~(94%)	93 (100%)	0	100	100
40	S	95/97~(98%)	95 (100%)	0	100	100
41	Т	78/82~(95%)	78 (100%)	0	100	100
42	U	90/97~(93%)	90 (100%)	0	100	100
43	V	76/84~(90%)	76 (100%)	0	100	100
44	W	83/88~(94%)	83 (100%)	0	100	100
45	Y	57/76~(75%)	57 (100%)	0	100	100
46	Ζ	45/53~(85%)	45 (100%)	0	100	100
47	1	48/55~(87%)	48 (100%)	0	100	100
48	2	50/52~(96%)	50 (100%)	0	100	100
49	3	48/73~(66%)	47 (98%)	1 (2%)	53	79
50	4	44/50 (88%)	44 (100%)	0	100	100



Mol	Chain	Analysed	analysed Rotameric Outliers		Percentiles		
51	5	44/48~(92%)	44 (100%)	0	100	100	
52	6	39/39~(100%)	39 (100%)	0	100	100	
53	7	54/56~(96%)	54 (100%)	0	100	100	
54	8	32/35~(91%)	32 (100%)	0	100	100	
All	All	3745/4674~(80%)	3741 (100%)	4 (0%)	93	98	

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	1	136	LYS
29	F	78	ARG
29	F	115	ARG
49	3	10	ARG

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such side chains are listed below:

Mol	Chain	Res	Type
35	Ν	27	ASN
44	W	67	ASN
35	Ν	126	ASN
38	Q	43	GLN
45	Y	58	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1512/1550~(97%)	340 (22%)	0
21	Х	71/76~(93%)	18 (25%)	0
22	W	8/21~(38%)	6~(75%)	0
24	А	2897/2932~(98%)	457 (15%)	29 (1%)
25	В	113/116~(97%)	12 (10%)	0
All	All	4601/4695~(97%)	833 (18%)	29~(0%)

5 of 833 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	а	9	G
1	a	17	U



Continued from previous page...

Mol	Chain	Res	Type
1	а	22	G
1	a	31	G
1	a	32	А

5 of 29 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	А	1468	G
24	А	2809	А
24	А	1530	G
24	А	2438	G
24	А	1528	G

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

7 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	Type	ne Chain Bes Link		who Chain Bog Link		Bo	Bond lengths			Bond angles		
WIOI	Moi Type Chain	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2		
21	G7M	х	46	21	20,26,27	2.64	4 (20%)	17,39,42	0.90	1 (5%)		
21	PSU	х	55	21	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)		
21	PSU	х	32	21	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)		
21	4SU	х	8	21	18,21,22	1.77	5 (27%)	26,30,33	2.39	6 (23%)		
21	5MU	х	54	21	19,22,23	1.36	5 (26%)	28,32,35	2.11	6 (21%)		
21	MIA	х	37	21	24,31,32	2.18	3 (12%)	26,44,47	2.51	8 (30%)		
21	PSU	х	39	21	18,21,22	1.28	2 (11%)	22,30,33	1.97	4 (18%)		

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
21	G7M	х	46	21	-	2/3/25/26	0/3/3/3
21	PSU	Х	55	21	-	0/7/25/26	0/2/2/2
21	PSU	Х	32	21	-	0/7/25/26	0/2/2/2
21	4SU	х	8	21	-	2/7/25/26	0/2/2/2
21	5MU	Х	54	21	-	0/7/25/26	0/2/2/2
21	MIA	Х	37	21	-	1/11/33/34	0/3/3/3
21	PSU	Х	39	21	-	0/7/25/26	0/2/2/2

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
21	Х	46	G7M	C8-N9	7.50	1.46	1.33
21	Х	37	MIA	C13-C14	7.10	1.52	1.32
21	Х	46	G7M	C8-N7	6.96	1.45	1.33
21	Х	37	MIA	C2-S10	-6.46	1.70	1.75
21	Х	8	4SU	C4-S4	-4.54	1.59	1.68

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
21	Х	37	MIA	C12-C13-C14	-8.40	110.80	127.14
21	Х	8	4SU	C4-N3-C2	-7.09	120.46	127.34
21	Х	39	PSU	N1-C2-N3	6.05	121.99	115.13
21	Х	8	4SU	C5-C4-N3	6.01	120.26	114.69
21	Х	32	PSU	N1-C2-N3	5.96	121.88	115.13

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	Х	37	MIA	C12-C13-C14-C16
21	Х	46	G7M	O4'-C4'-C5'-O5'
21	Х	8	4SU	C3'-C4'-C5'-O5'
21	Х	8	4SU	O4'-C4'-C5'-O5'
21	Х	46	G7M	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.



5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 428 ligands modelled in this entry, 427 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).

Mal	Type	o Chain Bog Link		Tink	Bond lengths			Bond angles		
WIOI	wor Type Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2	
57	GCP	v	503	55	27,34,34	1.40	5 (18%)	34,54,54	1.90	8 (23%)

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
57	GCP	v	503	55	-	5/15/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
57	V	503	GCP	C5-C6	3.75	1.47	1.41
57	V	503	GCP	PG-O3G	2.71	1.61	1.54
57	V	503	GCP	PG-O2G	2.66	1.61	1.54
57	V	503	GCP	C5-C4	2.18	1.46	1.40
57	V	503	GCP	PB-O3A	2.18	1.60	1.58

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
57	V	503	GCP	C2-N3-C4	4.81	120.86	115.36
57	V	503	GCP	C4-C5-C6	-3.87	117.10	120.80
57	V	503	GCP	C5-C6-N1	-3.82	118.21	123.43
57	V	503	GCP	C2-N1-C6	3.79	121.96	115.93



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
57	V	503	GCP	N3-C2-N1	-3.19	122.97	127.22

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	V	503	GCP	C5'-O5'-PA-O1A
57	V	503	GCP	O4'-C4'-C5'-O5'
57	V	503	GCP	C3'-C4'-C5'-O5'
57	V	503	GCP	C5'-O5'-PA-O3A
57	V	503	GCP	C5'-O5'-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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-42571. 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: 256



Y Index: 256



Z Index: 256

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: 255

Y Index: 244

Z Index: 178

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 3.5. 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 1018 $\rm nm^3;$ this corresponds to an approximate mass of 919 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.323 \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-42571 and PDB model 8UU8. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 3.5 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 (3.5).



9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 85% 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 (3.5) and Q-score for the entire model and for each chain.

\mathbf{Chain}	Atom inclusion	Q-score		
All	0.8460	0.4960		
1	0.8590	0.5500		
2	0.8820	0.5800		
3	0.3020	0.2860		
4	0.8910	0.5710		
5	0.8390	0.5660		
6	0.9360	0.6050		
7	0.9240	0.6010		
8	0.8910	0.5920		
А	0.9200	0.5500		
В	0.9080	0.4850		
C	0.8710	0.5900		
D	0.8960	0.5870		
Е	0.8740	0.5700		
F	0.5140	0.4000		
G	0.6820	0.4780		
Η	0.3860	0.3430		
Ι	0.1510	0.3370		
L	0.9260	0.5950		
Μ	0.8450	0.5760		
Ν	0.8600	0.5600		
О	0.8680	0.5810		
Р	0.8770	0.5780		
Q	0.7450	0.5010		
R	0.8400	0.5760		
S	0.9230	0.5940		
Т	0.9200	0.5940		
U	0.8840	0.5870		
V	0.8720	0.5720		
W	0.7820	0.5250		
Y	0.9120	0.5890		
Z	0.8730	0.5650		
a	0.8410	0.4110		
b	0.6710	0.4360		
с	0.5490	0.1920		



Chain	Atom inclusion	Q-score
d	0.8700	0.5170
е	0.8670	0.5350
f	0.7060	0.4520
g	0.3860	0.0340
h	0.8590	0.5290
i	0.6450	0.1130
j	0.6020	0.0820
k	0.7420	0.4800
1	0.8530	0.5560
m	0.4170	0.1220
n	0.6900	0.0940
О	0.7910	0.5200
р	0.8960	0.5470
q	0.8040	0.5060
r	0.8750	0.5140
s	0.2050	0.0830
t	0.8370	0.5190
V	0.7140	0.4890
W	0.3630	0.3800
X	0.1390	0.3140

