

Aug 10, 2023 – 06:12 pm BST

PDB ID	:	8BHJ
EMDB ID	:	EMD-16057
Title	:	Elongating E. coli 70S ribosome containing deacylated tRNA(iMet) in the P-
		site and Am6AA mRNA codon with cognate dipeptidyl-tRNA(Lys) in the
		A-site
Authors	:	Koziej, L.; Glatt, S.
Deposited on	:	2022-10-31
Resolution	:	2.81 Å(reported)
This is	a l	Full wwPDB EM Validation Report for a publicly released PDB entry.
		We welcome your comments at validation@mail.wwpdb.org
		A ugon muido is outilable at

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. dev 50
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	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.81 Å.

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



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM\ structures}\ (\#{ m Entries})$
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	А	273	99% •
2	В	209	100%
3	С	201	100%
4	D	179	99% •
5	Е	177	97%
6	F	149	99% ·
7	G	142	100%
8	Н	123	100%



Mol	Chain	Length	Quality of chain	
9	Ι	144	• 100%	
10	J	136	100%	
11	Κ	127	93%	7%
12	L	117	99%	
13	М	115	99%	
14	Ν	118	99%	
15	О	103	• 100%	
16	Р	110	100%	
17	Q	100	93%	7%
18	R	104	98%	•
19	S	94	• 100%	
20	Т	85	88%	12%
21	U	78	• 99%	
22	V	63	95%	5%
23	W	59	97%	·
24	a	57	96%	•
25	b	55	91%	• 7%
26	с	46	• 100%	
27	d	65	98%	•
28	е	38	100%	
29	f	241	37% 93%	7%
30	g	233	88%	12%
31	h	206	41%	
32	i	167	93%	7%
33	j	131	81%	19%
			Continued on n	$ext \ page$

WORLDWIDE PROTEIN DATA BANK

Mol	Chain	Length	Quality of chain	
34	k	179	16%	16%
01	n n	110	6%	1070
35	1	130	99%	
36	m	130	98%	·
37	n	103	96%	· ·
38	0	129	5% 91%	9%
39	n	124	6%	
00	Р	121	16%	
40	q	118	97%	•
41	r	101	99%	
42	s	89	9%	
43	t	82	16%	
44	u	84	10%	5%
45	V	75	21%	1.20/
10	v	10	24%	12 /0
46	W	92	85%	• 14%
47	x	87	99%	·
48	v	71	38%	
	J		•	
49	0	2904	82%	13% 5%
50	1	120	91%	9%
51	2	1542	6% 77%	23% •
52	3	30	27% 7% 67%	
53	4	77	26%	30%
54	5	76	5%	26%
04	0	10	50%	2070 •
55	6	2	50%	50%



2 Entry composition (i)

There are 55 unique types of molecules in this entry. The entry contains 237726 atoms, of which 95530 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues			AltConf	Trace				
1	А	271	Total 4236	C 1288	Н 2154	N 423	0 364	S 7	0	0

• Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues			AltConf	Trace				
2	В	208	Total 3170	C 976	Н 1611	N 287	O 292	$\frac{S}{4}$	0	0

• Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues			AltConf	Trace				
3	С	201	Total 3171	C 974	H 1619	N 283	O 290	${ m S}{ m 5}$	0	0

• Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	177	Total 2854	C 899	Н 1444	N 249	O 256	S 6	0	0

• Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues			AltConf	Trace				
5	Е	173	Total 2627	C 814	Н 1332	N 237	0 242	${ m S} { m 2}$	0	0

• Molecule 6 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues			AltConf	Trace				
6	F	149	Total 2259	C 699	Н 1148	N 197	0 214	S 1	0	0



• Molecule 7 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues			Atom	.s			AltConf	Trace
7	G	142	Total 2291	С 714	Н 1162	N 212	0 199	${f S}{4}$	0	0

• Molecule 8 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues			AltConf	Trace				
8	Н	123	Total 1970	C 593	Н 1023	N 181	0 167	S 6	0	0

• Molecule 9 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues			Atom	S			AltConf	Trace
9	Ι	144	Total 2182	$\begin{array}{c} \mathrm{C} \\ 654 \end{array}$	Н 1129	N 207	0 190	${ m S} { m 2}$	0	0

• Molecule 10 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues			Atom	IS			AltConf	Trace
10	J	136	Total 2231	C 686	Н 1157	N 205	0 177	S 6	0	0

• Molecule 11 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
11	K	118	Total 1934	C 585	Н 989	N 194	0 161	${f S}{5}$	0	0

• Molecule 12 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues		Α	toms			AltConf	Trace
12	L	116	Total 1815	C 552	Н 923	N 178	O 162	0	0

• Molecule 13 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
13	М	114	Total 1879	C 574	Н 962	N 179	O 163	${f S}$ 1	0	0

• Molecule 14 is a protein called 50S ribosomal protein L20.



Mol	Chain	Residues		A	Atoms			AltConf	Trace
14	Ν	117	Total 1966	C 604	H 1019	N 192	O 151	0	0

• Molecule 15 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues			Aton	ıs			AltConf	Trace
15	О	103	Total 1655	C 516	Н 839	N 153	0 145	${ m S} { m 2}$	0	0

• Molecule 16 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues			AltConf	Trace				
16	Р	110	Total 1779	C 532	Н 922	N 166	O 156	${ m S} { m 3}$	0	0

• Molecule 17 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues			Aton	ıs			AltConf	Trace
17	Q	93	Total 1545	C 466	Н 807	N 139	0 131	${ m S} { m 2}$	0	0

• Molecule 18 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues		A	toms			AltConf	Trace
18	R	102	Total 1610	C 492	Н 831	N 146	0 141	0	0

• Molecule 19 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
19	S	94	Total 1533	C 479	Н 780	N 137	0 134	${ m S} { m 3}$	0	0

• Molecule 20 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues			AltConf	Trace				
20	Т	75	Total 1165	$\begin{array}{c} \mathrm{C} \\ 355 \end{array}$	Н 593	N 116	O 100	S 1	0	0

• Molecule 21 is a protein called 50S ribosomal protein L28.



Mol	Chain	Residues			Atom	ıs			AltConf	Trace
21	U	77	Total 1277	C 388	Н 652	N 129	O 106	${ m S} { m 2}$	0	0

• Molecule 22 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues		A	Atom	s			AltConf	Trace
22	V	60	Total 1014	C 303	Н 523	N 96	O 91	S 1	0	0

• Molecule 23 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues		ŀ	AltConf	Trace				
23	W	57	Total 921	C 276	Н 482	N 86	O 75	${ m S} { m 2}$	0	0

• Molecule 24 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues		ŀ	Atom	s			AltConf	Trace
24	a	55	Total 879	C 263	Н 445	N 92	0 78	S 1	0	0

• Molecule 25 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues		At	oms			AltConf	Trace
25	b	51	Total 868	C 269	Н 451	N 76	0 72	0	0

• Molecule 26 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues		ŀ	Atom	s			AltConf	Trace
26	С	46	Total 795	C 228	Н 418	N 90	O 57	${ m S} { m 2}$	0	0

• Molecule 27 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues		_	AltConf	Trace				
27	d	64	Total 1077	C 323	Н 573	N 105	О 74	${ m S} { m 2}$	0	0

• Molecule 28 is a protein called 50S ribosomal protein L36.



Mol	Chain	Residues		ŀ	Atom	s			AltConf	Trace
28	е	38	Total 645	C 185	Н 343	N 65	0 48	${f S}$ 4	0	0

• Molecule 29 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues			Atoms	5			AltConf	Trace
29	f	224	Total 3533	C 1109	Н 1780	N 315	0 321	S 8	0	0

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

Mol	Chain	Residues			Atoms	5			AltConf	Trace
30	g	206	Total 3320	C 1028	Н 1696	N 305	O 288	${ m S} { m 3}$	0	0

• Molecule 31 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues			Atoms	5			AltConf	Trace
31	h	205	Total 3350	C 1026	Н 1707	N 315	O 298	$\frac{S}{4}$	0	0

• Molecule 32 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues			Atom	S			AltConf	Trace
32	i	155	Total 2329	C 711	Н 1185	N 216	0 211	S 6	0	0

• Molecule 33 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues			Atom	ns			AltConf	Trace
33	j	106	Total 1726	C 545	Н 864	N 156	0 154	${ m S} 7$	0	0

• Molecule 34 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues			Atom	IS			AltConf	Trace
34	k	151	Total 2419	C 735	Н 1238	N 227	0 215	${S \atop 4}$	0	0

• Molecule 35 is a protein called 30S ribosomal protein S8.



Mol	Chain	Residues			Atom	IS			AltConf	Trace
35	1	129	Total 2010	C 616	Н 1031	N 173	O 184	${ m S}{ m 6}$	0	0

• Molecule 36 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues			Atom	.s			AltConf	Trace
36	m	127	Total 2092	С 634	Н 1070	N 206	O 179	${ m S} { m 3}$	0	0

• Molecule 37 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues			Aton	ıs			AltConf	Trace
37	n	99	Total 1631	C 498	Н 836	N 152	O 144	S 1	0	0

• Molecule 38 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
38	О	117	Total 1764	C 540	Н 887	N 174	0 160	${ m S} { m 3}$	0	0

• Molecule 39 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues			Atom	S			AltConf	Trace
39	р	123	Total 1971	C 590	Н 1016	N 196	O 165	$\frac{S}{4}$	0	0

• Molecule 40 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
40	q	114	Total 1824	С 546	Н 941	N 178	O 156	${ m S} { m 3}$	0	0

• Molecule 41 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
41	r	100	Total 1649	C 499	Н 844	N 164	O 139	${ m S} { m 3}$	0	0

• Molecule 42 is a protein called 30S ribosomal protein S15.



Mol	Chain	Residues			Aton	ns			AltConf	Trace
42	s	88	Total 1448	C 439	Н 734	N 144	O 130	S 1	0	0

• Molecule 43 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues			Aton	ıs			AltConf	Trace
43	t	82	Total 1315	C 406	Н 666	N 128	0 114	S 1	0	0

• Molecule 44 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
44	u	80	Total 1339	C 411	Н 691	N 121	O 113	${ m S} { m 3}$	0	0

• Molecule 45 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues		_	Atom	s			AltConf	Trace
45	V	66	Total 1109	C 345	Н 565	N 102	O 96	S 1	0	0

• Molecule 46 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
46	W	79	Total 1302	C 408	Н 665	N 120	O 107	${ m S} { m 2}$	0	0

• Molecule 47 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
47	x	86	Total 1389	C 414	Н 719	N 138	0 115	${ m S} { m 3}$	0	0

• Molecule 48 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues		_	Atom	S			AltConf	Trace
48	У	70	Total 1219	C 366	H 629	N 125	O 98	S 1	0	0

• Molecule 49 is a RNA chain called 23S rRNA RRLG-RRNA.



Mol	Chain	Residues			Ato	ms			AltConf	Trace
49	0	2758	Total	С	Н	Ν	Ο	Р	0	Ο
45	0	2100	89005	26417	29786	10911	19134	2757	0	0

• Molecule 50 is a RNA chain called 5S rRNA.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
50	1	120	Total 3868	C 1144	Н 1302	N 468	O 835	Р 119	0	0

• Molecule 51 is a RNA chain called 16S rRNA RRSB-RRNA.

Mol	Chain	Residues			Ato	ns			AltConf	Trace
51	2	1534	Total 49480	C 14681	H 16563	N 6041	O 10661	Р 1534	0	0

• Molecule 52 is a RNA chain called mRNA.

Mol	Chain	Residues			Aton	ıs			AltConf	Trace
52	3	10	Total 325	C 98	H 109	N 41	0 67	Р 10	0	0

• Molecule 53 is a RNA chain called Deacylated P-site tRNA(fMet).

Mol	Chain	Residues			At	oms				AltConf	Trace
53	4	77	Total 2468	С 734	Н 826	N 297	0 534	Р 76	S 1	0	0

• Molecule 54 is a RNA chain called Dipeptidyl A-site tRNA(Lys).

Mol	Chain	Residues			At	oms				AltConf	Trace
54	5	76	Total	С	Η	Ν	Ο	Р	\mathbf{S}	0	0
04	0	10	2456	729	831	283	537	75	1		0

• Molecule 55 is a protein called fMet-Lys dipeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace	
55	6	2	Total 37	C 12	H 18	N 3	O 3	S 1	0	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: 50S ribosomal protein L2

Chain A:	99%	I
MET A2 K28 S272 LYS		
• Molecule 2: 50S ribosomal protein L3		
Chain B:	100%	
M1 K208 ALA		
• Molecule 3: 50S ribosomal protein L4		
Chain C:	100%	
There are no outlier residues recorded f	or this chain.	
• Molecule 4: 50S ribosomal protein L5		
16%		
Chain D:	99% •	'
MET A.2 K.9 D10 D10 H18 H23 A54 A54 A54 A54 A54 K47 A54 K47 K47 K47 K47 K47 K73 K78 K78 K78 K78 K78 K78 K78 K80 K86	A107 1111 1111 1111 1111 1111 1111 1111 1111 1111 1111 1111 1111 1111 1112 1123 1123 1140 1141 1142 1144 1145 1145 1145 1147 1147 1143 1144 1145 1145 1147 1143 1145 1145 1147 1143 1143 1144 1145 1147 1148 1149 1144 1145 1145 1145 1145 1145 1146 1147 1148 1149 <	D174 F175
• Molecule 5: 50S ribosomal protein L6		
Chain E:	97%	
MET S2 446 446 446 446 446 446 446 446 446 44		

• Molecule 6: 50S ribosomal protein L9



	70%	
Chain F:	99%	
M1 140 K41 K41 K41 F43 F45 F45 F46 F46 F46 F46 F46 F46 F46 F46 F46 F46	A52 E53 E55 A56 A56 A56 A59 A64 A67 A67 A67 A67 A67 A67 A67 A74 C72 A74 C72 A74 C72 A74 A74 A74 A74 A74 A74 A77 A77 A77 A77	180 A81 A81 A84 A84 A84 A84 G85 E87 G88 F91 F91 F91 G92 G92 G92 G92 G95 F91 F91 F91 F91 F94 F91 F94 F97
D98 199 A100 D101 A102 A102 A105 A105 G107 V108 C107 V108	A111 K112 E114 V115 L117 P118 N119 0120 C120 C122 C122 C122 C122 C122 C122	V138 F139 A140 X144 V142 V142 V144 V145 F143 V145 F143 F148 F149
• Molecule 7: 50S ribos	somal protein L13	
Chain G:	100%	
There are no outlier res	sidues recorded for this chain.	
• Molecule 8: 50S ribos	somal protein L14	
Chain H:	100%	
There are no outlier res	sidues recorded for this chain.	
• Molecule 9: 50S ribos	somal protein L15	
Chain I:	100%	
• Molecule 10: 50S ribo	osomal protein L16	
Chain J:	100%	
There are no outlier res	sidues recorded for this chain.	
• Molecule 11: 50S ribo	osomal protein L17	
Chain K:	93%	7%
M R18 SER SER CLU ALA ALA ALA ALA ALA CLU		
• Molecule 12: 50S ribo	osomal protein L18	
Chain L:	99%	
MET D2 F117		
• Molecule 13: 50S ribo	osomal protein L19	



Chain M: 99% ·
\bullet Molecule 14: 50S ribosomal protein L20
Chain N: 99%
MET A118
• Molecule 15: 50S ribosomal protein L21
Chain O: 100%
• Molecule 16: 50S ribosomal protein L22
Chain P: 100%
◆ ◆ Solution of the second s
\bullet Molecule 17: 50S ribosomal protein L23
Chain Q: 93% 7%
HI AND
\bullet Molecule 18: 50S ribosomal protein L24
Chain R: 98% .
MET A2 ME3 4 G8 4 L103 L71 03
\bullet Molecule 19: 50S ribosomal protein L25
Chain S:
◆ V V V V V V



• Molecule 20:	: 50S ribosomal protein L27	
Chain T:	88%	12%
MET ALA ALA LYS LYS ALA GLY SER SER	484 GLU	
• Molecule 21:	: 50S ribosomal protein L28	
Chain U:	99%	.
MET S2 K77 Y78		
• Molecule 22:	: 50S ribosomal protein L29	
Chain V:	95%	5%
MET K2 A61 GLY ALA		
• Molecule 23:	: 50S ribosomal protein L30	
Chain W:	97%	
MET A2 E58 GLU		
• Molecule 24:	: 50S ribosomal protein L32	
Chain a:	96%	
MET A2 A56 LYS		
• Molecule 25:	: 50S ribosomal protein L33	
Chain b:	91%	• 7%
MET ALA LYS G4 G4 R28 K53 K53 K53		
• Molecule 26:	: 50S ribosomal protein L34	
Chain c:	100%	



	•
M1	K46

• Molecule 27: 50S ribosomal protein L35

Chain d: 98% .

• Molecule 28: 50S ribosomal protein L36

Chain e: 100%

There are no outlier residues recorded for this chain.

 \bullet Molecule 29: 30S ribosomal protein S2





1200 P205 A206 A206 A206 A206 A206 A227 A213 A226 A227 A226 A226 A227 A226 A226 A227 A26 A206 A

 \bullet Molecule 30: 30S ribosomal protein S3





- Molecule 32: 30S ribosomal protein S5 Chain i: 93% 7% MET ALA HIS HIS ILE CLU CLU CLV CLV CLV CLV CLV CLV CLV • Molecule 33: 30S ribosomal protein S6 13% Chain j: 81% 19% ASP GLU GLU GLU GLU GLU ARG ARG PHE ARSP PHE ARSP CLU GLU GLU ARSP GLU ARSP GLV GLU GLU GLU GLU • Molecule 34: 30S ribosomal protein S7 16% Chain k: 84% 16% • Molecule 35: 30S ribosomal protein S8 Chain 1: 99% • Molecule 36: 30S ribosomal protein S9 8% Chain m: 98% ME1 AL/ GLU • Molecule 37: 30S ribosomal protein S10 14% Chain n: 96% GLN
- Molecule 38: 30S ribosomal protein S11



• Molecule 39: 30S ribosomal protein S12 • Molecule 40: 30S ribosomal protein S13 • Molecule 40: 30S ribosomal protein S13 • Molecule 41: 30S ribosomal protein S14 • Molecule 42: 30S ribosomal protein S15 • Molecule 43: 30S ribosomal protein S16	Chain o:	91%	9%
• Molecule 39: 30S ribosomal protein S12 Chain p: • 6^{56} • Molecule 40: 30S ribosomal protein S13 Chain q: • 6^{56} • 6^{56}	MET ALA LYS LYS ALA ALA ALA ARG LYS K14 K13 K13 K13 K13 K14 K14	E76 A103 C104 V129 V129	
Chain p:	• Molecule 39: 30S ribose	omal protein S12	
Molecule 40: 30S ribosomal protein S13 187 Chain q: 97% Molecule 41: 30S ribosomal protein S14 137 Chain r: 99% Molecule 42: 30S ribosomal protein S15 9% Molecule 42: 30S ribosomal protein S15 9% Molecule 43: 30S ribosomal protein S16 16% Chain t: 10% Molecule 44: 30S ribosomal protein S16 16% Chain t: 10% Molecule 44: 30S ribosomal protein S16 16% Molecule 44: 30S ribosomal protein S17 10%	Chain p:	99%	
Molecule 40: 30S ribosomal protein S13 16% 97% 98 97% Molecule 41: 30S ribosomal protein S14 13% 99% Chain r: 99% 98 98 98 Molecule 42: 30S ribosomal protein S15 9% 9% 9% 9% Molecule 42: 30S ribosomal protein S15 9% 99% Molecule 43: 30S ribosomal protein S16 10% Molecule 43: 30S ribosomal protein S16 10% Molecule 44: 30S ribosomal protein S17 10%	MET A2 R14 E70 E70 C75 R121 P122 R121 P122 K123 A124		
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	• Molecule 40: 30S ribose	omal protein S13	
$\begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \end{array} \\ \end{array} \\ \end{array} \\ \end{array} \\ \end{array} \\ \begin{array}{c} \begin{array}{c} \begin{array}{c} \end{array} \\ \begin{array}{c} \begin{array}{c} \end{array} \\ \end{array} \\ \end{array} \\ \end{array} \\ \end{array} \\ \begin{array}{c} \begin{array}{c} \end{array} \\ \begin{array}{c} \begin{array}{c} \end{array} \\ \end{array} $	Chain q:	97%	
 Molecule 41: 30S ribosomal protein S14 Chain r: 99% Molecule 42: 30S ribosomal protein S15 Molecule 42: 30S ribosomal protein S15 9% Chain s: 99% Molecule 43: 30S ribosomal protein S16 16% Chain t: 100% Molecule 44: 30S ribosomal protein S17 	MET A2 R3 R3 A35 A35 A35 A35 A35 A35 A35 A35 A35 A3	R71 M75 M75 M81 M81 D82 C86 C86 C86 C86 C86 C86 C86 C86 C86 C86	
13% Chain r: 99% $Molecule 42: 30S ribosomal protein S15$ $9%$ Chain s: 99% $Molecule 43: 30S ribosomal protein S16$ $16%$ Chain t: 100% $Molecule 44: 30S ribosomal protein S16$ $16%$ Chain t: 100% $Molecule 44: 30S ribosomal protein S17$	• Molecule 41: 30S riboso	omal protein S14	
 Molecule 42: 30S ribosomal protein S15 Molecule 43: 30S ribosomal protein S16 Molecule 43: 30S ribosomal protein S16 Molecule 44: 30S ribosomal protein S17 	Chain r:	99%	
 Molecule 42: 30S ribosomal protein S15 9% Chain s: 99% Molecule 43: 30S ribosomal protein S16 16% Chain t: 100% Molecule 44: 30S ribosomal protein S17 10% 	MET A2 E10 E10 A13 A25 E26 L16 A25 E26 L27 A35 A36 S37	M42 K47 61 M61 M101	
9% Chain s: 99% Molecule 43: 30S ribosomal protein S16 16% Molecule 44: 30S ribosomal protein S17 10% Thain u:	• Molecule 42: 30S ribose	omal protein S15	
 A A A A A A A A A A A A A A A A A A A	Chain s:	99%	
 Molecule 43: 30S ribosomal protein S16 Chain t: 100% Molecule 44: 30S ribosomal protein S17 10% 	MET 22 018 A19 N20 D21 E45 E45 E45 E45 E45 E45 E45 E45		
16% Chain t: 100% Image: State	• Molecule 43: 30S ribose	omal protein S16	
 Molecule 44: 30S ribosomal protein S17 Chain u: 	Chain t:	100%	
• Molecule 44: 30S ribosomal protein S17	M1 L6 S44 E45 E45 E47 E47 E47 E48 Q63 Q63	K76 N 79 A 81 A 82 A 82	
10%	• Molecule 44: 30S ribose	omal protein S17	
Sham u. 95% 5%	Chain u:	95%	5%





• Molecule 45: 30S ribosomal protein S18













4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24054	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	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.320	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.091	Depositor
Map size (Å)	440.32, 440.32, 440.32	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	$0.86, 0.86, \overline{0.86}$	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: T6A, U8U, 4SU, 5MU, 6MZ, OMC, FME, H2U

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	Bo	ond lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.27	0/2121	0.58	0/2852	
2	В	0.27	0/1580	0.54	0/2127	
3	С	0.26	0/1571	0.52	0/2113	
4	D	0.26	0/1434	0.53	0/1926	
5	Ε	0.27	0/1315	0.53	0/1783	
6	F	0.24	0/1122	0.49	0/1515	
7	G	0.28	0/1152	0.52	0/1551	
8	Н	0.27	0/956	0.57	0/1279	
9	Ι	0.26	0/1062	0.59	0/1413	
10	J	0.27	0/1093	0.60	0/1460	
11	Κ	0.27	0/958	0.61	0/1281	
12	L	0.27	0/902	0.56	0/1209	
13	М	0.26	0/929	0.57	0/1242	
14	Ν	0.30	0/960	0.58	0/1278	
15	0	0.28	0/829	0.56	0/1107	
16	Р	0.26	0/864	0.55	0/1156	
17	Q	0.26	0/744	0.53	0/994	
18	R	0.26	0/787	0.52	0/1051	
19	S	0.26	0/766	0.51	0/1025	
20	Т	0.26	0/579	0.56	0/767	
21	U	0.26	0/635	0.61	0/848	
22	V	0.25	0/492	0.53	0/655	
23	W	0.25	0/443	0.57	0/593	
24	a	0.25	0/440	0.61	0/588	
25	b	0.25	0/424	0.50	0/565	
26	с	0.26	0/380	0.66	0/498	
27	d	0.27	0/513	0.60	$0/\overline{676}$	
28	е	0.27	0/303	0.59	0/397	
29	f	0.24	0/1784	0.48	0/2403	
30	g	0.26	0/1651	0.56	0/2225	
31	h	0.26	0/1665	0.54	0/2227	
32	i	0.27	0/1157	0.54	0/1557	



Mol Chain		Bo	ond lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
33	j	0.25	0/881	0.51	0/1189	
34	k	0.24	0/1195	0.56	0/1602	
35	1	0.26	0/989	0.53	0/1326	
36	m	0.25	0/1034	0.59	0/1375	
37	n	0.24	0/805	0.57	0/1089	
38	0	0.25	0/893	0.55	0/1205	
39	р	0.25	0/969	0.59	0/1300	
40	q	0.24	0/892	0.59	0/1193	
41	r	0.25	0/817	0.56	0/1088	
42	s	0.25	0/722	0.55	0/964	
43	t	0.25	0/659	0.57	0/884	
44	u	0.24	0/657	0.54	0/881	
45	V	0.25	0/553	0.55	0/742	
46	W	0.25	0/652	0.55	0/877	
47	Х	0.27	0/676	0.52	0/895	
48	у	0.27	0/598	0.60	0/792	
49	0	0.38	0/66326	0.79	7/103471~(0.0%)	
50	1	0.31	0/2869	0.75	0/4474	
51	2	0.32	2/36859~(0.0%)	0.79	5/57501~(0.0%)	
52	3	1.04	0/215	0.84	0/330	
53	4	0.63	0/1766	0.72	0/2753	
54	5	0.79	0/1663	0.77	0/2588	
55	6	0.29	0/8	0.27	0/8	
All	All	0.35	2/154309~(0.0%)	0.73	12/230888~(0.0%)	

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	2	1393	U	O3'-P	-5.82	1.54	1.61
51	2	1400	С	O3'-P	5.62	1.67	1.61

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
51	2	178	С	N3-C2-O2	-6.31	117.48	121.90
51	2	754	С	C2-N1-C1'	6.03	125.43	118.80
51	2	178	С	N1-C2-O2	5.83	122.40	118.90
49	0	1605	С	N1-C2-O2	5.71	122.33	118.90
49	0	1313	U	C2-N1-C1'	5.66	124.50	117.70
49	0	1605	С	N3-C2-O2	-5.66	117.94	121.90
49	0	12	U	C2-N1-C1'	5.65	124.48	117.70
51	2	1466	С	N3-C2-O2	-5.57	118.00	121.90



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
49	0	2321	U	C2-N1-C1'	5.29	124.05	117.70
49	0	274	С	N1-C2-O2	5.22	122.03	118.90
49	0	481	G	O4'-C1'-N9	5.22	112.38	108.20
51	2	993	G	C4-N9-C1'	5.01	133.02	126.50

There are no chirality outliers.

There are no planarity outliers.

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
1	А	269/273~(98%)	260 (97%)	9 (3%)	0	100	100
2	В	206/209~(99%)	195 (95%)	11 (5%)	0	100	100
3	С	199/201~(99%)	190 (96%)	9 (4%)	0	100	100
4	D	175/179~(98%)	160 (91%)	15 (9%)	0	100	100
5	Ε	171/177~(97%)	165 (96%)	6 (4%)	0	100	100
6	F	147/149~(99%)	135~(92%)	12 (8%)	0	100	100
7	G	140/142~(99%)	137 (98%)	3 (2%)	0	100	100
8	Н	121/123~(98%)	112 (93%)	9 (7%)	0	100	100
9	Ι	142/144~(99%)	134 (94%)	8 (6%)	0	100	100
10	J	134/136~(98%)	121 (90%)	13 (10%)	0	100	100
11	K	116/127~(91%)	107 (92%)	9 (8%)	0	100	100
12	L	114/117~(97%)	109 (96%)	5 (4%)	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
13	М	112/115~(97%)	110 (98%)	2(2%)	0	100	100
14	Ν	115/118~(98%)	113 (98%)	2(2%)	0	100	100
15	О	101/103~(98%)	98~(97%)	3 (3%)	0	100	100
16	Р	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
17	Q	91/100 (91%)	86 (94%)	5~(6%)	0	100	100
18	R	100/104~(96%)	93~(93%)	7 (7%)	0	100	100
19	S	92/94~(98%)	89~(97%)	3(3%)	0	100	100
20	Т	73/85~(86%)	70~(96%)	3~(4%)	0	100	100
21	U	75/78~(96%)	73~(97%)	2(3%)	0	100	100
22	V	58/63~(92%)	57~(98%)	1 (2%)	0	100	100
23	W	55/59~(93%)	53~(96%)	2(4%)	0	100	100
24	a	53/57~(93%)	51 (96%)	2(4%)	0	100	100
25	b	49/55~(89%)	48 (98%)	1 (2%)	0	100	100
26	с	44/46~(96%)	44 (100%)	0	0	100	100
27	d	62/65~(95%)	58 (94%)	4 (6%)	0	100	100
28	е	36/38~(95%)	36 (100%)	0	0	100	100
29	f	222/241~(92%)	199 (90%)	23~(10%)	0	100	100
30	g	204/233~(88%)	188 (92%)	16 (8%)	0	100	100
31	h	203/206~(98%)	196 (97%)	7(3%)	0	100	100
32	i	153/167~(92%)	143 (94%)	10 (6%)	0	100	100
33	j	104/131~(79%)	100 (96%)	4 (4%)	0	100	100
34	k	149/179~(83%)	140 (94%)	9 (6%)	0	100	100
35	1	127/130~(98%)	118 (93%)	9~(7%)	0	100	100
36	m	125/130~(96%)	116 (93%)	9~(7%)	0	100	100
37	n	97/103~(94%)	91 (94%)	6 (6%)	0	100	100
38	О	115/129~(89%)	107 (93%)	8 (7%)	0	100	100
39	р	121/124 (98%)	114 (94%)	7 (6%)	0	100	100
40	q	112/118~(95%)	101 (90%)	11 (10%)	0	100	100
41	r	98/101~(97%)	93~(95%)	5 (5%)	0	100	100
42	s	86/89~(97%)	85 (99%)	1 (1%)	0	100	100

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100

100

0



3(4%)

77 (96%)

80/82 (98%)

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
44	u	78/84~(93%)	72~(92%)	6 (8%)	0	100 100
45	v	64/75~(85%)	64 (100%)	0	0	100 100
46	W	77/92~(84%)	69~(90%)	8 (10%)	0	100 100
47	х	84/87~(97%)	82~(98%)	2(2%)	0	100 100
48	У	68/71~(96%)	66~(97%)	2 (3%)	0	100 100
All	All	5525/5839~(95%)	5227 (95%)	298 (5%)	0	100 100

There are no Ramachandran outliers to report.

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
1	А	216/218~(99%)	216 (100%)	0	100	100
2	В	164/164~(100%)	164 (100%)	0	100	100
3	\mathbf{C}	165/165~(100%)	165~(100%)	0	100	100
4	D	148/150~(99%)	148 (100%)	0	100	100
5	Ε	134/138~(97%)	133~(99%)	1 (1%)	84	95
6	F	114/114~(100%)	113 (99%)	1 (1%)	78	93
7	G	116/116~(100%)	116 (100%)	0	100	100
8	Н	104/104~(100%)	104 (100%)	0	100	100
9	Ι	103/103~(100%)	103 (100%)	0	100	100
10	J	109/109~(100%)	109 (100%)	0	100	100
11	Κ	98/103~(95%)	98 (100%)	0	100	100
12	L	86/87~(99%)	86 (100%)	0	100	100
13	М	99/100~(99%)	99 (100%)	0	100	100
14	Ν	89/90~(99%)	89 (100%)	0	100	100
15	Ο	84/84~(100%)	84 (100%)	0	100	100
16	Р	93/93~(100%)	93~(100%)	0	100	100



Mol	Chain	Analysed	Rotameric	Outliers	Perc	cer	ntiles
17	Q	80/84~(95%)	80 (100%)	0	100		100
18	R	83/85~(98%)	83 (100%)	0	100		100
19	S	78/78~(100%)	78 (100%)	0	100]	100
20	Т	57/63~(90%)	57 (100%)	0	100		100
21	U	67/68~(98%)	67 (100%)	0	100		100
22	V	54/55~(98%)	54 (100%)	0	100		100
23	W	47/49~(96%)	47 (100%)	0	100		100
24	a	46/48~(96%)	46 (100%)	0	100		100
25	b	46/49~(94%)	45 (98%)	1 (2%)	52		81
26	с	38/38~(100%)	38 (100%)	0	100		100
27	d	51/52~(98%)	51 (100%)	0	100		100
28	е	34/34~(100%)	34 (100%)	0	100		100
29	f	186/199 (94%)	186 (100%)	0	100]	100
30	g	170/190~(90%)	170 (100%)	0	100		100
31	h	172/173~(99%)	172 (100%)	0	100]	100
32	i	118/126 (94%)	118 (100%)	0	100	T	100
33	j	92/112~(82%)	92 (100%)	0	100		100
34	k	124/147~(84%)	124 (100%)	0	100		100
35	1	104/105~(99%)	104 (100%)	0	100		100
36	m	105/107~(98%)	105 (100%)	0	100		100
37	n	87/90~(97%)	87 (100%)	0	100]	100
38	0	90/99~(91%)	90 (100%)	0	100		100
39	р	103/104 (99%)	103 (100%)	0	100		100
40	q	92/96~(96%)	92 (100%)	0	100		100
41	r	83/84~(99%)	83 (100%)	0	100		100
42	s	76/77~(99%)	76 (100%)	0	100		100
43	t	65/65~(100%)	65 (100%)	0	100		100
44	u	74/78~(95%)	74 (100%)	0	100		100
45	v	57/65~(88%)	57 (100%)	0	100		100
46	W	70/79~(89%)	69 (99%)	1 (1%)	67		89
47	х	65/66~(98%)	65 (100%)	0	100	1	100



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Mol	Chain	Analysed	Rotameric	Outliers	Pe	erce	ntile	\mathbf{s}
48	У	60/61~(98%)	60 (100%)	0	1	.00	100	
55	6	$1/1 \ (100\%)$	1 (100%)	0	1	.00	100	
All	All	4597/4765~(96%)	4593 (100%)	4 (0%)		93	98	

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

Mol	Chain	Res	Type
5	Ε	69	ARG
6	F	41	LYS
25	b	28	ARG
46	W	6	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
32	i	122	ASN
47	Х	48	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
49	0	2754/2904~(94%)	376 (13%)	7 (0%)
50	1	119/120~(99%)	11 (9%)	0
51	2	1534/1542~(99%)	320 (20%)	51 (3%)
52	3	8/30~(26%)	1 (12%)	0
53	4	76/77~(98%)	19~(25%)	1 (1%)
54	5	74/76~(97%)	18 (24%)	3(4%)
All	All	4565/4749~(96%)	745 (16%)	62 (1%)

All (745) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
49	0	10	А
49	0	12	U
49	0	13	А
49	0	34	U
49	0	35	G
49	0	45	G
49	0	46	G



Mol	Chain	Res	Type
49	0	63	А
49	0	71	А
49	0	74	А
49	0	75	G
49	0	99	U
49	0	101	А
49	0	102	U
49	0	103	А
49	0	118	А
49	0	119	А
49	0	120	U
49	0	125	А
49	0	135	U
49	0	139	U
49	0	140	С
49	0	163	С
49	0	181	А
49	0	196	А
49	0	199	A
49	0	201	С
49	0	215	G
49	0	216	А
49	0	222	А
49	0	233	А
49	0	248	G
49	0	249	С
49	0	266	G
49	0	272	А
49	0	275	С
49	0	277	G
49	0	278	A
49	0	281	С
49	0	287	G
49	0	302	С
49	0	304	U
49	0	311	A
49	0	318	С
49	0	323	С
49	0	329	G
49	0	330	A
49	0	361	G
49	0	362	А



Mol	Chain	Res	Type
49	0	372	G
49	0	386	G
49	0	396	G
49	0	404	А
49	0	405	U
49	0	411	G
49	0	412	А
49	0	413	С
49	0	424	G
49	0	429	А
49	0	441	U
49	0	449	А
49	0	467	G
49	0	481	G
49	0	490	С
49	0	491	G
49	0	494	G
49	0	505	А
49	0	509	С
49	0	510	С
49	0	530	G
49	0	532	А
49	0	538	А
49	0	545	U
49	0	547	A
49	0	548	G
49	0	557	С
49	0	563	А
49	0	573	U
49	0	574	А
49	0	575	A
49	0	585	G
49	0	603	A
49	0	613	A
49	0	614	A
49	0	615	U
49	0	634	C
49	0	637	A
49	0	639	U
49	0	645	С
49	0	647	G
49	0	686	U



Mol	Chain	Res	Type
49	0	707	G
49	0	714	U
49	0	724	U
49	0	730	А
49	0	747	U
49	0	758	С
49	0	764	А
49	0	766	U
49	0	775	G
49	0	776	G
49	0	779	U
49	0	782	А
49	0	783	А
49	0	784	G
49	0	785	G
49	0	805	G
49	0	812	С
49	0	827	U
49	0	828	U
49	0	837	С
49	0	846	U
49	0	859	G
49	0	878	А
49	0	879	G
49	0	881	G
49	0	896	А
49	0	910	А
49	0	914	G
49	0	915	С
49	0	931	U
49	0	932	U
49	0	934	U
49	0	946	С
49	0	959	A
49	0	961	С
49	0	974	G
49	0	983	A
49	0	996	A
49	0	997	G
49	0	1009	A
49	0	1012	U
49	0	1013	С



Mol	Chain	Res	Type
49	0	1022	G
49	0	1024	G
49	0	1026	G
49	0	1027	А
49	0	1033	U
49	0	1034	G
49	0	1043	С
49	0	1046	А
49	0	1047	G
49	0	1110	G
49	0	1112	G
49	0	1119	U
49	0	1125	G
49	0	1132	U
49	0	1135	С
49	0	1136	G
49	0	1142	А
49	0	1171	G
49	0	1173	U
49	0	1174	U
49	0	1176	U
49	0	1180	U
49	0	1187	G
49	0	1206	G
49	0	1210	G
49	0	1211	С
49	0	1212	G
49	0	1226	А
49	0	1238	G
49	0	1250	G
49	0	1253	А
49	0	1255	U
49	0	1256	G
49	0	1268	А
49	0	1271	G
49	0	1272	A
49	0	1286	А
49	0	1300	G
49	0	1301	А
49	0	1322	A
49	0	1341	G
49	0	1345	С



Mol	Chain	Res	Type
49	0	1365	А
49	0	1379	U
49	0	1395	А
49	0	1412	U
49	0	1416	G
49	0	1417	С
49	0	1418	G
49	0	1420	А
49	0	1428	С
49	0	1429	G
49	0	1435	G
49	0	1452	G
49	0	1455	G
49	0	1460	U
49	0	1482	G
49	0	1483	G
49	0	1490	А
49	0	1493	С
49	0	1495	А
49	0	1497	U
49	0	1508	А
49	0	1509	А
49	0	1510	G
49	0	1515	А
49	0	1516	G
49	0	1533	С
49	0	1535	А
49	0	1560	G
49	0	1567	G
49	0	1569	А
49	0	1571	А
49	0	1578	U
49	0	1583	A
49	0	1584	U
49	0	1585	С
49	0	1587	G
49	0	1607	С
49	0	1608	А
49	0	1618	A
49	0	1647	U
49	0	1648	U
49	0	1674	G



Mol	Chain	Res	Type
49	0	1676	А
49	0	1715	G
49	0	1717	А
49	0	1729	U
49	0	1730	С
49	0	1737	G
49	0	1738	G
49	0	1744	А
49	0	1756	G
49	0	1758	U
49	0	1764	С
49	0	1773	А
49	0	1775	U
49	0	1776	G
49	0	1780	А
49	0	1786	А
49	0	1787	А
49	0	1800	С
49	0	1808	А
49	0	1811	G
49	0	1816	С
49	0	1827	U
49	0	1829	А
49	0	1872	А
49	0	1873	G
49	0	1886	U
49	0	1906	G
49	0	1913	А
49	0	1917	U
49	0	1919	А
49	0	1929	G
49	0	1930	G
49	0	1934	C
49	0	1936	A
49	0	1937	A
49	0	1938	A
49	0	1955	U
49	0	1964	G
49	0	1967	C
49	0	1970	A
49	0	1971	U
49	0	1972	G



Mol	Chain	Res	Type
49	0	1991	U
49	0	1993	U
49	0	1997	С
49	0	2006	С
49	0	2023	С
49	0	2031	А
49	0	2033	А
49	0	2034	U
49	0	2043	С
49	0	2053	G
49	0	2055	С
49	0	2056	G
49	0	2060	А
49	0	2061	G
49	0	2062	A
49	0	2069	G
49	0	2093	G
49	0	2186	G
49	0	2187	U
49	0	2188	U
49	0	2190	G
49	0	2194	U
49	0	2204	G
49	0	2211	А
49	0	2225	А
49	0	2227	А
49	0	2238	G
49	0	2239	G
49	0	2247	А
49	0	2251	G
49	0	2279	G
49	0	2283	С
49	0	2287	A
49	0	2288	А
49	0	2289	G
49	0	2297	A
49	0	2305	U
49	0	2307	G
49	0	2308	G
49	0	$2\overline{309}$	A
49	0	2312	U
49	0	2322	А



Mol	Chain	Res	Type
49	0	2325	G
49	0	2333	А
49	0	2345	G
49	0	2347	С
49	0	2367	G
49	0	2383	G
49	0	2385	С
49	0	2402	U
49	0	2403	С
49	0	2406	А
49	0	2422	С
49	0	2425	А
49	0	2429	G
49	0	2430	А
49	0	2434	А
49	0	2435	А
49	0	2441	U
49	0	2448	А
49	0	2474	U
49	0	2475	С
49	0	2476	А
49	0	2478	А
49	0	2482	А
49	0	2491	U
49	0	2492	U
49	0	2502	G
49	0	2503	А
49	0	2505	G
49	0	2507	С
49	0	2508	G
49	0	2518	А
49	0	2529	G
49	0	2534	А
49	0	2538	С
49	0	2547	А
49	0	2566	А
49	0	2567	G
49	0	2572	A
49	0	2573	С
49	0	2582	G
49	0	2600	А
49	0	2602	А



Mol	Chain	Res	Type
49	0	2603	G
49	0	2608	G
49	0	2609	U
49	0	2613	U
49	0	2615	U
49	0	2629	U
49	0	2662	А
49	0	2689	U
49	0	2690	U
49	0	2714	G
49	0	2726	А
49	0	2733	А
49	0	2748	А
49	0	2752	С
49	0	2778	А
49	0	2780	G
49	0	2791	G
49	0	2799	А
49	0	2811	G
49	0	2820	А
49	0	2832	U
49	0	2835	А
49	0	2849	U
49	0	2850	А
49	0	2867	G
49	0	2880	С
49	0	2883	А
49	0	2884	U
49	0	2885	G
49	0	2886	А
49	0	2887	A
49	0	2894	G
49	0	2895	G
50	1	21	G
50	1	35	С
50	1	41	G
50	1	44	G
50	1	47	С
50	1	89	U
50	1	90	С
50	1	105	G
50	1	108	А



Mol	Chain	Res	Type
50	1	109	А
50	1	116	G
51	2	2	А
51	2	6	G
51	2	8	А
51	2	9	G
51	2	22	G
51	2	32	А
51	2	38	G
51	2	39	G
51	2	41	G
51	2	46	G
51	2	47	С
51	2	48	С
51	2	51	А
51	2	54	С
51	2	66	А
51	2	71	А
51	2	77	А
51	2	80	А
51	2	81	А
51	2	84	U
51	2	85	U
51	2	86	G
51	2	104	G
51	2	108	G
51	2	120	А
51	2	121	U
51	2	122	G
51	2	129	А
51	2	131	A
51	2	144	G
51	2	151	A
51	2	156	С
51	2	162	A
51	2	163	С
51	2	167	A
51	2	168	G
51	2	169	С
51	2	171	A
51	2	173	U
51	2	179	А



Mol	Chain	Res	Type
51	2	183	С
51	2	184	G
51	2	186	C
51	2	188	С
51	2	189	А
51	2	190	А
51	2	195	А
51	2	199	А
51	2	209	U
51	2	210	С
51	2	211	G
51	2	212	G
51	2	234	C
51	2	245	U
51	2	247	G
51	2	251	G
51	2	252	U
51	2	263	А
51	2	266	G
51	2	267	С
51	2	274	А
51	2	279	А
51	2	281	G
51	2	282	А
51	2	283	U
51	2	286	С
51	2	289	G
51	2	299	G
51	2	304	U
51	2	309	А
51	2	314	C
51	2	316	С
51	2	321	A
51	2	328	С
51	2	330	C
51	2	332	G
51	2	342	С
51	2	345	C
51	2	346	G
51	2	348	G
51	2	352	С
51	2	354	G



Mol	Chain	Res	Type
51	2	367	U
51	2	368	U
51	2	372	С
51	2	384	G
51	2	390	U
51	2	397	A
51	2	404	G
51	2	406	G
51	2	409	U
51	2	412	А
51	2	413	G
51	2	414	А
51	2	422	С
51	2	423	G
51	2	429	U
51	2	438	U
51	2	448	А
51	2	464	U
51	2	481	G
51	2	484	G
51	2	486	U
51	2	493	А
51	2	495	А
51	2	496	A
51	2	506	G
51	2	509	А
51	2	511	С
51	2	512	U
51	2	514	С
51	2	518	С
51	2	524	G
51	2	532	А
51	2	547	A
51	2	548	G
51	2	554	A
51	2	559	A
51	2	560	А
51	2	564	C
51	2	567	G
51	2	569	С
51	2	571	U
51	2	572	А



Mol	Chain	Res	Type
51	2	573	А
51	2	576	С
51	2	577	G
51	2	583	А
51	2	587	G
51	2	600	А
51	2	603	U
51	2	640	А
51	2	653	U
51	2	665	А
51	2	674	G
51	2	687	А
51	2	698	G
51	2	703	G
51	2	704	A
51	2	707	U
51	2	718	А
51	2	722	G
51	2	723	U
51	2	724	G
51	2	733	G
51	2	734	G
51	2	742	G
51	2	777	А
51	2	785	G
51	2	793	U
51	2	794	А
51	2	802	А
51	2	811	С
51	2	815	A
51	2	817	С
51	2	830	G
51	2	832	G
51	2	840	C
51	2	842	U
51	2	843	U
51	2	846	G
51	2	851	G
51	2	858	G
51	2	872	A
51	2	873	A
51	2	882	C



Mol	Chain	Res	Type
51	2	885	G
51	2	889	A
51	2	890	G
51	2	891	U
51	2	914	А
51	2	926	G
51	2	927	G
51	2	934	С
51	2	935	A
51	2	937	A
51	2	942	G
51	2	956	U
51	2	960	U
51	2	961	U
51	2	963	G
51	2	965	U
51	2	966	G
51	2	967	С
51	2	969	А
51	2	971	G
51	2	975	A
51	2	976	G
51	2	977	А
51	2	981	U
51	2	983	А
51	2	984	С
51	2	990	С
51	2	992	U
51	2	993	G
51	2	1002	G
51	2	1004	A
51	2	1005	A
51	2	1006	G
51	2	1008	U
51	2	1012	A
51	2	1018	G
51	2	1024	G
51	2	1025	U
51	2	1026	G
51	2	1030	U
51	2	1033	G
51	2	1034	G



Mol	Chain	Res	Type
51	2	1035	А
51	2	1036	А
51	2	1037	С
51	2	1041	G
51	2	1043	G
51	2	1044	А
51	2	1054	С
51	2	1066	С
51	2	1075	U
51	2	1079	G
51	2	1094	G
51	2	1095	U
51	2	1101	А
51	2	1102	А
51	2	1117	А
51	2	1118	U
51	2	1119	С
51	2	1124	G
51	2	1126	U
51	2	1130	А
51	2	1132	С
51	2	1136	С
51	2	1137	С
51	2	1138	G
51	2	1139	G
51	2	1142	G
51	2	1147	С
51	2	1152	А
51	2	1158	С
51	2	1159	U
51	2	1169	А
51	2	1170	А
51	2	1177	G
51	2	1178	G
51	2	1183	U
51	2	1184	G
51	2	1191	А
51	2	1196	A
51	2	1197	A
51	2	1200	С
51	2	1202	U
51	2	1212	U



Mol	Chain	Res	Type	
51	2	1213	А	
51	2	1214	С	
51	2	1215	G	
51	2	1216	А	
51	2	1221	G	
51	2	1222	G	
51	2	1227	А	
51	2	1231	G	
51	2	1236	А	
51	2	1238	А	
51	2	1241	G	
51	2	1247	U	
51	2	1257	А	
51	2	1258	G	
51	2	1268	G	
51	2	1275	A	
51	2	1279	G	
51	2	1280	А	
51	2	1287	А	
51	2	1294	G	
51	2	1297	G	
51	2	1300	G	
51	2	1302	С	
51	2	1317	С	
51	2	1318	А	
51	2	1319	А	
51	2	1321	U	
51	2	1322	С	
51	2	1329	А	
51	2	1331	G	
51	2	1335	U	
51	2	1337	G	
51	2	1338	G	
51	2	1347	G	
51	2	1348	U	
51	2	1359	С	
51	2	1360	А	
51	2	1362	A	
51	2	1363	A	
51	2	1364	U	
51	2	1370	G	
51	2	1374	А	



Mol	Chain	Res	Type
51	2	1375	А
51	2	1378	С
51	2	1379	G
51	2	1391	U
51	2	1394	А
51	2	1398	А
51	2	1400	С
51	2	1401	G
51	2	1441	А
51	2	1442	G
51	2	1446	А
51	2	1453	G
51	2	1459	G
51	2	1469	С
51	2	1478	U
51	2	1487	G
51	2	1492	А
51	2	1494	G
51	2	1497	G
51	2	1503	А
51	2	1504	G
51	2	1506	U
51	2	1513	А
51	2	1517	G
51	2	1519	А
51	2	1529	G
51	2	1530	G
51	2	1534	А
52	3	14	U
53	4	8	G
53	4	11	G
53	4	15	С
53	4	16	С
$\overline{53}$	4	18	G
53	4	19	G
$\overline{53}$	4	22	G
53	4	23	С
53	4	25	С
53	4	26	G
53	4	30	G
53	4	35	A
53	4	38	A



Mol	Chain	Res	Type
53	4	41	С
53	4	44	А
53	4	53	G
53	4	55	U
53	4	70	G
53	4	76	А
54	5	4	U
54	5	8	U
54	5	13	С
54	5	14	А
54	5	16	H2U
54	5	17	H2U
54	5	20	H2U
54	5	22	G
54	5	23	А
54	5	25	С
54	5	33	U
54	5	42	А
54	5	50	С
54	5	51	А
54	5	57	G
54	5	63	U
54	5	69	A
54	5	73	А

All (62) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
49	0	277	G
49	0	546	U
49	0	895	U
49	0	1026	G
49	0	2193	G
49	0	2307	G
49	0	2481	G
51	2	1	А
51	2	80	А
51	2	83	С
51	2	130	А
51	2	178	С
51	2	188	С
51	2	210	С



Mol	Chain	Res	Type
51	2	251	G
51	2	281	G
51	2	315	А
51	2	345	С
51	2	422	С
51	2	428	G
51	2	463	U
51	2	485	U
51	2	495	А
51	2	559	А
51	2	575	G
51	2	602	А
51	2	703	G
51	2	792	А
51	2	839	С
51	2	842	U
51	2	845	А
51	2	890	G
51	2	960	U
51	2	982	U
51	2	992	U
51	2	1024	G
51	2	1040	U
51	2	1053	G
51	2	1117	А
51	2	1125	U
51	2	1136	С
51	2	1137	С
51	2	1151	А
51	2	1157	А
51	2	1182	G
51	2	1183	U
51	2	1190	G
51	2	1201	A
51	2	1230	С
51	2	1256	А
51	2	1317	С
51	2	1320	C
51	2	1337	G
51	2	1347	G
51	2	1399	C
51	2	1440	U



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Mol	Chain	Res	Type
51	2	1441	А
51	2	1452	С
53	4	10	А
54	5	13	С
54	5	15	G
54	5	21	А

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

11 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	Dec	Tink	Bo	Bond lengths			ond ang	les
	туре	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
55	FME	6	1	55	8,9,10	0.93	0	7,9,11	1.32	1 (14%)
54	H2U	5	17	54	18,21,22	0.98	2 (11%)	21,30,33	1.38	3 (14%)
53	4SU	4	7	53	18,21,22	1.74	4 (22%)	26,30,33	2.26	5 (19%)
54	U8U	5	34	54,52	19,24,25	1.76	3 (15%)	23,34,37	1.32	3 (13%)
54	H2U	5	20	54	18,21,22	0.99	2 (11%)	21,30,33	1.37	3 (14%)
53	OMC	4	32	53	19,22,23	0.99	2 (10%)	26,31,34	0.77	0
52	6MZ	3	20	54,52	18,25,26	1.75	4 (22%)	16,36,39	2.07	3 (18%)
54	T6A	5	37	54	27,34,35	0.98	0	29,49,52	2.70	9 (31%)
54	H2U	5	16	54	18,21,22	0.97	2 (11%)	21,30,33	1.36	3 (14%)
54	5MU	5	54	54	19,22,23	1.33	4 (21%)	28,32,35	2.12	7 (25%)
53	5MU	4	54	53	19,22,23	1.44	6 (31%)	28,32,35	2.07	7 (25%)

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
55	FME	6	1	55	-	4/7/9/11	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	H2U	5	17	54	-	3/7/38/39	0/2/2/2
53	4SU	4	7	53	-	2/7/25/26	0/2/2/2
54	U8U	5	34	54,52	-	2/9/28/29	0/2/2/2
54	H2U	5	20	54	-	5/7/38/39	0/2/2/2
53	OMC	4	32	53	-	0/9/27/28	0/2/2/2
52	6MZ	3	20	54,52	-	0/5/27/28	0/3/3/3
54	T6A	5	37	54	-	5/19/41/42	0/3/3/3
54	H2U	5	16	54	-	1/7/38/39	0/2/2/2
54	5MU	5	54	54	-	0/7/25/26	0/2/2/2
53	5MU	4	54	53	-	0/7/25/26	0/2/2/2

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	5	34	U8U	C2-S2	-5.55	1.59	1.67
52	3	20	6MZ	C6-N6	4.91	1.43	1.35
53	4	7	4SU	C4-S4	-4.58	1.59	1.68
54	5	34	U8U	C4-N3	-3.42	1.32	1.38
53	4	7	4SU	C4-N3	-3.28	1.34	1.37
54	5	54	5MU	C4-N3	-2.97	1.33	1.38
53	4	54	5MU	C6-C5	2.84	1.39	1.34
52	3	20	6MZ	C5-C4	-2.82	1.33	1.40
53	4	54	5MU	C4-N3	-2.78	1.33	1.38
53	4	32	OMC	C5-C4	-2.56	1.37	1.42
54	5	54	5MU	C6-N1	-2.50	1.33	1.38
54	5	16	H2U	C2-N3	-2.49	1.33	1.38
54	5	17	H2U	C2-N3	-2.48	1.33	1.38
53	4	7	4SU	C5-C4	-2.48	1.39	1.42
54	5	54	5MU	C2-N3	-2.47	1.33	1.38
54	5	20	H2U	C2-N3	-2.46	1.33	1.38
53	4	54	5MU	C4-C5	2.45	1.48	1.44
52	3	20	6MZ	C6-N1	-2.43	1.30	1.34
53	4	32	OMC	C6-N1	-2.29	1.32	1.38
53	4	54	5MU	C6-N1	-2.24	1.34	1.38
52	3	20	6MZ	C9-N6	-2.24	1.41	1.45
54	5	34	U8U	C2-N3	-2.23	1.32	1.37
53	4	54	5MU	C2-N3	-2.23	1.34	1.38
54	5	54	5MU	C6-C5	2.18	1.38	1.34
53	4	7	4SU	C2-N3	-2.15	1.34	1.38
54	5	17	H2U	C4-N3	-2.10	1.34	1.37
53	4	54	5MU	C2-N1	2.09	1.41	1.38



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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
54	5	16	H2U	C4-N3	-2.08	1.34	1.37
54	5	20	H2U	C4-N3	-2.06	1.34	1.37

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
54	5	37	T6A	N6-C10-N11	8.96	126.28	113.76
53	4	7	4SU	C4-N3-C2	-7.12	120.43	127.34
54	5	37	T6A	C2-N1-C6	6.72	122.35	116.59
53	4	7	4SU	C5-C4-N3	5.67	119.95	114.69
52	3	20	6MZ	N3-C2-N1	-5.63	119.87	128.68
54	5	54	5MU	C4-N3-C2	-5.31	120.47	127.35
54	5	54	5MU	N3-C2-N1	5.18	121.77	114.89
53	4	54	5MU	C4-N3-C2	-5.17	120.66	127.35
53	4	54	5MU	N3-C2-N1	5.11	121.68	114.89
54	5	37	T6A	N6-C6-N1	4.91	125.29	118.72
53	4	7	4SU	N3-C2-N1	4.53	120.90	114.89
54	5	54	5MU	C5-C4-N3	4.44	119.10	115.31
53	4	54	5MU	C5-C4-N3	4.42	119.08	115.31
52	3	20	6MZ	C2-N1-C6	4.26	120.24	116.59
54	5	20	H2U	C4-N3-C2	-4.16	122.34	125.79
54	5	17	H2U	C4-N3-C2	-4.09	122.40	125.79
54	5	16	H2U	C4-N3-C2	-4.05	122.43	125.79
54	5	34	U8U	O4-C4-C5	-3.92	119.13	124.96
54	5	37	T6A	O10-C10-N6	-3.90	117.02	123.62
53	4	54	5MU	C5-C6-N1	-3.86	119.37	123.34
53	4	7	4SU	C5-C4-S4	-3.84	119.52	124.47
54	5	54	5MU	O4-C4-C5	-3.72	120.59	124.90
54	5	34	U8U	C5-C4-N3	3.68	120.14	114.97
54	5	54	5MU	C5-C6-N1	-3.67	119.56	123.34
54	5	37	T6A	N3-C2-N1	-3.57	123.11	128.68
53	4	54	5MU	O4-C4-C5	-3.55	120.79	124.90
52	3	20	6MZ	C1'-N9-C4	-3.41	120.66	126.64
54	5	37	T6A	O10-C10-N11	-3.26	116.68	122.62
55	6	1	FME	C-CA-N	2.94	115.04	109.73
54	5	54	5MU	O2-C2-N1	-2.86	118.98	122.79
54	5	16	H2U	C5-C4-N3	2.77	119.77	116.65
54	5	17	H2U	C5-C4-N3	2.77	119.75	116.65
54	5	20	H2U	C5-C4-N3	2.72	119.70	116.65
54	5	37	T6A	C4-C5-N7	-2.50	106.80	109.40
53	4	7	4SU	O2-C2-N1	-2.48	119.49	122.79
53	4	54	5MU	O2-C2-N1	-2.40	119.59	122.79



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
54	5	20	H2U	C5-C6-N1	-2.31	103.99	111.61
54	5	37	T6A	C14-C12-C13	-2.21	106.42	110.19
54	5	17	H2U	C5-C6-N1	-2.16	104.50	111.61
54	5	34	U8U	C5-C6-N1	-2.14	120.03	122.91
54	5	54	5MU	C5M-C5-C4	2.09	121.07	118.77
54	5	37	T6A	C12-N11-C10	-2.05	118.53	121.94
54	5	16	H2U	C5-C6-N1	-2.00	105.02	111.61
53	4	54	5MU	C5M-C5-C4	2.00	120.97	118.77

There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
54	5	17	H2U	O4'-C1'-N1-C2
54	5	17	H2U	O4'-C1'-N1-C6
54	5	20	H2U	O4'-C1'-N1-C2
54	5	20	H2U	O4'-C1'-N1-C6
54	5	34	U8U	N-C-C5-C4
54	5	34	U8U	N-C-C5-C6
54	5	37	T6A	C13-C12-C14-O14
54	5	37	T6A	C13-C12-C14-C15
55	6	1	FME	O1-CN-N-CA
55	6	1	FME	CB-CA-N-CN
55	6	1	FME	N-CA-CB-CG
54	5	37	T6A	C13-C12-N11-C10
53	4	7	4SU	O4'-C4'-C5'-O5'
54	5	37	T6A	N11-C12-C14-O14
53	4	7	4SU	C3'-C4'-C5'-O5'
54	5	16	H2U	C4'-C5'-O5'-P
54	5	20	H2U	C4'-C5'-O5'-P
55	6	1	FME	C-CA-CB-CG
54	5	37	T6A	N11-C12-C14-C15
54	5	20	H2U	O4'-C4'-C5'-O5'
54	5	17	H2U	O4'-C4'-C5'-O5'
54	5	20	H2U	C3'-C4'-C5'-O5'

All (22) torsion outliers are listed below:

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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-16057. 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: 256





Z Index: 256

6.2.2 Raw map



X Index: 256

Y 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



6.3.2 Raw map



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 0.091. 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.



Mask visualisation (i) 6.6

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

$emd_{16057}msk_{1.map}$ (i) 6.6.1





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 852 nm^3 ; this corresponds to an approximate mass of 769 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 0.356 ${\rm \AA^{-1}}$



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 0.356 $\mathrm{\AA^{-1}}$



8.2 Resolution estimates (i)

$\begin{bmatrix} Bosolution ostimato (Å) \end{bmatrix}$	Estim	Estimation criterion (FSC cut-off)			
resolution estimate (A)	0.143	0.5	Half-bit		
Reported by author	2.81	-	-		
Author-provided FSC curve	2.81	3.20	2.87		
Unmasked-calculated*	4.01	7.30	4.24		

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.01 differs from the reported value 2.81 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-16057 and PDB model 8BHJ. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.091 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 (0.091).



9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.091) and Q-score for the entire model and for each chain.

\mathbf{Chain}	Atom inclusion	$\mathbf{Q} extsf{-score}$
All	0.8610	0.5220
0	0.9500	0.5940
1	0.9170	0.5240
2	0.8280	0.4510
3	0.9210	0.5690
4	0.6350	0.3770
5	0.8590	0.5250
6	0.6840	0.5850
А	0.9470	0.6260
В	0.9350	0.6200
\mathbf{C}	0.8990	0.5860
D	0.6310	0.3250
E	0.8130	0.5030
F	0.2580	0.2330
G	0.9400	0.6180
Н	0.9330	0.6180
Ι	0.9170	0.6090
J	0.9290	0.6050
K	0.9560	0.6350
L	0.8420	0.5160
М	0.9120	0.5970
Ν	0.9360	0.6300
Ο	0.9020	0.5870
Р	0.9080	0.6090
Q	0.8780	0.5670
R	0.8880	0.5750
S	0.8620	0.5680
<u> </u>	0.9260	0.6160
U	0.9170	0.5940
V	0.8560	0.5410
W	0.8990	0.5970
a	0.9310	0.6270
b	0.8340	0.5570
С	0.9490	0.6340
d	0.9290	0.6270



Chain	Atom inclusion	Q-score
е	0.9250	0.6150
f	0.4800	0.2730
g	0.7830	0.4600
h	0.4570	0.2530
i	0.8160	0.4560
j	0.6770	0.3780
k	0.5880	0.2950
1	0.7300	0.4130
m	0.7090	0.3860
n	0.6920	0.3860
0	0.7470	0.4250
р	0.8280	0.5250
q	0.6270	0.3080
r	0.7260	0.4300
S	0.7170	0.4180
t	0.6600	0.3750
u	0.7030	0.3950
V	0.6080	0.3660
W	0.5750	0.3230
X	0.7680	0.4280
y	0.4340	0.2750

