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PDB ID	:	6FXC
EMDB ID	:	EMD-3637
Title	:	The cryo-EM structure of hibernating 100S ribosome dimer from pathogenic
		Staphylococcus aureus
Authors	:	Matzov, D.; Aibara, S.; Zimmerman, E.; Bashan, A.; Kidmose, R.; Amunts,
		A.; Yonath, A.
Deposited on	:	2018-03-08
Resolution	:	6.76 Å(reported)
This is	a I	Full wwPDB EM Validation 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:

:	0.0.1.dev43
:	4.02b-467
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	1.9.9
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	2.31.2
	: : : : :

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 6.76 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.



Motrie	Whole archive	EM structures		
WIEUTIC	$(\# { m Entries})$	$(\# { m Entries})$		
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	Aa	1539	5% 68%	30%	•					
1	Ba	1539	5%	30%	•					
2	Ab	226	64%							
2	Bb	226	64%							
3	Ac	202	73%	•						
3	Bc	202	73%	-						
4	Ad	198	41%		•					
4	Bd	198	41%		•					



Conti	nued fron	n previous	page
Mol	Chain	Length	Quality of chain
			74%
5	Ae	156	99% •
			74%
5	Be	156	99% ·
			59%
6	At	95	99% .
C	DC	05	59%
0	BI	95	99% •
7	۸œ	159	08%
1	Ag	152	100%
7	Bσ	152	100%
- 1	D ₅	102	51%
8	Ah	131	98%
		101	51%
8	Bh	131	98%
			55%
9	Ai	127	97%
			55%
9	Bi	127	97% •
			56%
10	Aj	97	99% •
1.0	.		56%
10	Bj	97	99% .
11	A 1	114	54%
	AK	114	100%
11	DI-	114	54%
	DK	114	100%
12	A1	135	020/
12		100	66%
12	Bl	135	98%
		100	49%
13	Am	121	85% • 14%
			49%
13	Bm	121	85% • 14%
			22%
14	An	60	97% .
	-		22%
14	Bn	60	97% •
1.5			40%
15	Ao	88	99% •
15	B ₂	00	40%
10	DO	00	99% • 42%
16	Δp	80	
10	- rp	03	<u>42%</u>
16	Bn	89	98%
	24		52%
17	Aq	80	100%
l		1	



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Mol	Chain	Length	Quality of chain					
	D		54%					
17	Вq	80	100%					
18	Ar	54	%eC					
10		01	59%	· · ·				
18	Br	54	98%	·				
10	٨	0.0	32%					
19	As	80	99%	•				
19	Bs	80	00%					
	2.0		33%					
20	At	81	99%	•				
00	D	01	33%					
20	Bt	81	99% 94%	•				
21	Au	52	100%					
			94%					
21	Bu	52	100%					
00	۸	100	57%					
22	AV	190	<u> </u>	• 15%				
22	Bv	190	82%	• 15%				
			7%					
23	AA	2923	70% 27%					
-0.2	DA	2022	7%					
20	DA	2920	6%	27% ••				
24	AB	115	82%	17% •				
			6%					
24	BB	115	81%	17% ·				
25	AC	274	56%					
20	110	214	56%	•				
25	BC	274	99%	•				
			33%					
26	AD	215	99%	•				
26	BD	215	00%					
20	DD	210	46%					
27	AE	206	100%					
	DE	20.0	46%					
27	BE	206	100%					
28	AF	175	QQ%					
			59%					
28	BF	175	99%	•				
		175	55%					
- 29	AG	1/5	99%	•				
29	BG	175	99%	•				



Continue contract c	nued fron	n previous j	page
Mol	Chain	Length	Quality of chain
20	A T T	145	27%
30	AH	145	99% ·
30	BH	145	99%
		100	64%
31	Al	122	97% .
31	BI	122	97%
			47%
32	AJ	146	97% .
32	BJ	146	97%
		105	36%
33	AK	137	99%
33	BK	137	99%
	A T	100	31%
34	AL	120	99%
34	BL	120	99%
		110	30%
35	AM	119	96%
35	BM	119	97%
	A 3 T	114	46%
36	AN	114	98% •
36	BN	114	98% •
	10	110	20%
37	AO	116	99% ·
37	BO	116	99%
	4.D	100	42%
38	AP	102	<u> </u>
38	BP	102	98% •
	10	110	41%
39	AQ	112	<u> </u>
39	BQ	112	99%
10	AD	00	31%
40	AR	89	<u> </u>
40	BR	89	98%
41	AC	109	52%
41	AS	103	99% •
41	BS	103	99%
40	٨٣	0.4	76%
42	AT	94	• •



Mol	Chain	Length	Quality of chain
		0	76%
42	BT	94	99% .
43	AU	82	18% 95% 5%
43	BU	82	95% 5%
44	AV	58	98% •
44	BV	58	98%
45	AW	67	48%
45	BW	67	48%
46	AX	58	62%
46	BX	58	62%
47	۸V	50	90%
47	AI	- 59	90%
47	BY	59	100%
48	AZ	48	100%
48	ΒZ	48	100%
49	A1	47	83%
49	B1	47	83%
50	A2	43	30%
50	B2	43	30%
51	A3	64	27%
51	B3	64	27%
52	A4	37	97%
52	B4	37	97%





2 Entry composition (i)

There are 52 unique types of molecules in this entry. The entry contains 281510 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 Aa	Δρ	1530	Total	С	Ν	Ο	Р	0	0
	Ла	1009	32969	14719	6017	10694	1539	0	0
1 Ba	Ba	1530	Total	С	Ν	О	Р	0	0
		1009	32969	14719	6017	10694	1539	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2 Ab	Ab	226	Total	С	Ν	0	S	0	0
	AU	220	1813	1156	314	335	8	0	
2 Bb	226	Total	С	Ν	0	S	0	0	
	DD	DD	DD 220	1813	1156	314	335	8	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3 Ac	Δο	202	Total	С	Ν	0	S	0	0
	AC	202	1501	945	284	271	1	0	0
3 Bo	Bo	202	Total	С	Ν	0	S	0	0
	DC	202	1501	945	284	271	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Ad	198	Total 1497	C 952	N 275	O 268	${S \over 2}$	0	0
4	Bd	198	Total 1497	C 952	N 275	O 268	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

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



Mol	Chain	Residues		At	oms		AltConf	Trace	
5	Δο	156	Total	С	Ν	0	S	0	0
0	AC	100	1145	723	211	209	2	0	0
5	Bo	156	Total	С	Ν	0	S	0	0
0	De	150	1145	723	211	209	2	0	0

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

Mol	Chain	Residues		At	oms		AltConf	Trace	
6	Λf	05	Total	С	Ν	0	S	0	0
0	AI	95	778	493	138	145	2	0	0
6	Df	05	Total	С	Ν	0	S	0	0
0	DI	90	778	493	138	145	2	0	0

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

Mol	Chain	Residues		At	oms		AltConf	Trace	
7	Ag	152	Total 1161	C 722	N 218	0 217	${s \atop 4}$	0	0
7	Bg	152	Total 1161	C 722	N 218	0 217	${S \atop 4}$	0	0

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

Mol	Chain	Residues		At	oms		AltConf	Trace	
8	Ab	121	Total	С	Ν	0	S	0	0
0	АП	131	1026	650	183	189	4	0	0
8	Bh	121	Total	С	Ν	0	S	0	0
0	DII	131	1026	650	183	189	4	0	0

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

Mol	Chain	Residues		At	oms		AltConf	Trace	
0	Δ;	197	Total	С	Ν	0	S	0	0
9	Al	121	922	576	179	166	1	0	
0	D;	197	Total	С	Ν	0	S	0	0
9	DI	127	922	576	179	166	1	0	0

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

Mol	Chain	Residues		At	oms			AltConf	Trace
10	Aj	97	Total 752	C 475	N 140	0 136	S 1	0	0



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Mol	Chain	Residues		At	oms			AltConf	Trace
10	Bj	97	Total 752	$\begin{array}{c} \mathrm{C} \\ 475 \end{array}$	N 140	0 136	S 1	0	0

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

Mol	Chain	Residues		At	oms		AltConf	Trace	
11	۸ŀ	114	Total	С	Ν	0	S	0	0
	ЛК	114	810	498	151	159	2	0	0
11	Bŀ	114	Total	С	Ν	Ο	S	0	0
	DK	114	810	498	151	159	2	0	

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

Mol	Chain	Residues		At	oms		AltConf	Trace	
10	A1	125	Total	С	Ν	0	S	0	0
12	AI	155	1037	646	211	178	2	0	0
10	DI	125	Total	С	Ν	0	S	0	0
		199	1037	646	211	178	2	0	

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

Mol	Chain	Residues		Ato	ms		AltConf	Trace
13	Am	104	Total 727	C 453	N 139	O 135	0	0
13	Bm	104	Total 727	C 453	N 139	O 135	0	0

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

Mol	Chain	Residues		Ato	\mathbf{ms}		AltConf	Trace	
14	An	60	Total	C	N	0	S	0	0
			487	307	98	((б		
1/	Bn	60	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
14	DII	00	487	307	98	77	5	0	0

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

Mol	Chain	Residues		At	oms		AltConf	Trace	
15	Δο	<u> </u>	Total	С	Ν	0	S	0	0
10	10 A0	00	723	448	150	124	1	0	
15	Bo	00	Total	С	Ν	0	S	0	0
10	DO	00	723	448	150	124	1	0	0



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

Mol	Chain	Residues		At	oms	AltConf	Trace		
16	Δn	80	Total	С	Ν	Ο	S	0	0
10	лр	03	694	436	128	129	1	0	0
16	Bn	80	Total	С	Ν	Ο	\mathbf{S}	0	0
10	Ър	09	694	436	128	129	1	0	0

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

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
17	Aq	80	Total 621	C 392	N 112	O 117	0	0
17	Bq	80	Total 621	C 392	N 112	O 117	0	0

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

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
18	Ar	54	Total 446	C 284	N 86	0 74	$\frac{S}{2}$	0	0
18	Br	54	Total 446	C 284	N 86	0 74	2 S 2	0	0

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

Mol	Chain	Residues		At	oms		AltConf	Trace	
10	Δα	80	Total	С	Ν	0	S	0	0
19	AS	80	636	410	113	111	2	0	0
10	Be	80	Total	С	Ν	0	S	0	0
19	DS	80	636	410	113	111	2	0	0

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
20	Δ+	81	Total	С	Ν	Ο	S	0	0
20	110	01	591	358	117	115	1	0	0
20	B+	81	Total	С	Ν	0	\mathbf{S}	0	0
		01	591	358	117	115	1		

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



Mol	Chain	Residues		Aton	ıs		AltConf	Trace
21	Au	52	Total 400	C 249	N 79	O 72	0	0
21	Bu	52	Total 400	C 249	N 79	O 72	0	0

• Molecule 22 is a protein called Ribosome hibernation promotion factor.

Mol	Chain	Residues		At	oms	AltConf	Trace		
22	٨	169	Total	С	Ν	0	S	0	0
	AV	102	1333	835	242	254	2	0	0
20	Bu	169	Total	С	Ν	0	S	0	0
	DV	102	1333	835	242	254	2	0	0

 $\bullet\,$ Molecule 23 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues				AltConf	Trace		
93	ΔΔ	2005	Total	С	Ν	Ο	Р	0	0
20	20 AA 29	2900	62277	27803	11387	20182	2905	0	0
93	ΒΛ	2005	Total	С	Ν	О	Р	0	0
20	DA	2900	62277	27803	11387	20182	2905	0	0

• Molecule 24 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues		A		AltConf	Trace		
24	٨B	115	Total	С	Ν	Ο	Р	0	0
24	AD	110	2445	1094	436	801	114	0	0
24	BB	115	Total	С	Ν	Ο	Р	0	0
24		110	2445	1094	436	801	114	0	0

• Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues		Ate	AltConf	Trace			
25	AC	274	Total 2094	C 1303	N 415	0 371	${f S}{5}$	0	0
25	BC	274	Total 2094	C 1303	N 415	О 371	${ m S}{ m 5}$	0	0

• Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues		Ate	AltConf	Trace			
26	AD	215	Total 1627	C 1018	N 299	O 305	${ m S}{ m 5}$	0	0



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Mol	Chain	Residues		At	AltConf	Trace			
26	BD	215	Total 1627	C 1018	N 299	O 305	${ m S}{ m 5}$	0	0

• Molecule 27 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues		At	oms		AltConf	Trace	
97	٨F	206	Total	С	Ν	0	S	0	0
21	AL	200	1572	986	288	296	2	0	0
97	BE	206	Total	С	Ν	0	S	0	0
21	DĽ	200	1572	986	288	296	2	0	0

• Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues		At	oms		AltConf	Trace	
28	ΔF	175	Total	С	Ν	Ο	S	0	0
20	Ar	175	1325	837	227	255	6	0	0
20	PE	175	Total	С	Ν	0	S	0	0
20	DF	175	1325	837	227	255	6	0	0

• Molecule 29 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues		At	oms		AltConf	Trace	
20		175	Total	С	Ν	0	S	0	0
29	AG	175	1263	790	239	231	3	0	0
20	BC	175	Total	С	Ν	0	S	0	0
29	DG	170	1263	790	239	231	3	0	U

• Molecule 30 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues		At	oms		AltConf	Trace	
30	ΔН	145	Total	С	Ν	Ο	\mathbf{S}	0	0
50	7111	140	1143	714	208	218	3	0	0
30	ВН	145	Total	С	Ν	Ο	\mathbf{S}	0	0
- 30	DII	140	1143	714	208	218	3	0	0

• Molecule 31 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues		At	oms		AltConf	Trace	
21	ΔΤ	199	Total	С	Ν	Ο	S	0	0
51	AI	122	918	572	174	168	4	0	0
21	BI	199	Total	С	Ν	0	S	0	0
51	DI	122	918	572	174	168	4	0	0



• Molecule 32 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues		At	oms		AltConf	Trace	
30	ΛΤ	146	Total	С	Ν	0	S	0	0
52	AJ	140	1086	674	214	197	1	0	0
30	BI	146	Total	С	Ν	0	S	0	0
32	DJ	140	1086	674	214	197	1		

• Molecule 33 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues		At	oms		AltConf	Trace	
33	AK	137	Total	С	N	0	S	0	0
			1071	689	203	175	4		
33	BK	137	Total	С	Ν	Ο	\mathbf{S}	0	0
00	DI	107	1071	689	203	175	4	0	0

• Molecule 34 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues		At	oms		AltConf	Trace	
34	ΔT	120	Total	С	Ν	0	S	0	0
- 54	AL	120	932	576	182	173	1	0	0
34	BI	120	Total	С	Ν	0	S	0	0
- 54	DL	120	932	576	182	173	1	0	0

• Molecule 35 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues		At	oms		AltConf	Trace	
35	АМ	110	Total	С	Ν	0	S	0	0
- 55	AM	119	891	557	174	159	1	0	0
35	BM	110	Total	С	Ν	Ο	S	0	0
- 55	DIVI	119	891	557	174	159	1	0	0

• Molecule 36 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues		Ato	ms		AltConf	Trace
36	AN	114	Total	С	Ν	Ο	0	0
50	AIN	114	889	563	175	151	0	0
26	ΡN	114	Total	С	Ν	Ο	0	0
- 50	DN	114	889	563	175	151	0	U

• Molecule 37 is a protein called 50S ribosomal protein L20.



Mol	Chain	Residues		At	oms		AltConf	Trace	
37	AO	116	Total 942	C 593	N 189	O 156	$\frac{S}{4}$	0	0
37	BO	116	Total 942	C 593	N 189	0 156	$\frac{S}{4}$	0	0

• Molecule 38 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues		At	oms		AltConf	Trace	
20	٨D	109	Total	С	Ν	0	S	0	0
30	AF	102	790	503	142	144	1	0	0
20	DD	109	Total	С	Ν	0	S	0	0
- 30	DF	102	790	503	142	144	1	0	0

• Molecule 39 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues		At	oms	AltConf	Trace		
39	AQ	112	Total 854	С 534	N 164	0 153	${ m S} { m 3}$	0	0
39	BQ	112	Total 854	С 534	N 164	0 153	${ m S} { m 3}$	0	0

• Molecule 40 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues		At	oms	AltConf	Trace		
40	٨B	80	Total	С	Ν	Ο	S	0	0
40 An	09	715	453	127	131	4	0		
40	BB	80	Total	С	Ν	0	S	0	0
40 1	DR	DR 89	715	453	127	131	4	0	0

• Molecule 41 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues		At	oms	AltConf	Trace			
41	٨S	103	Total	С	Ν	Ο	\mathbf{S}	0	0	
41 A5	105	770	486	142	141	1	0			
41	BS	103	Total	С	Ν	Ο	\mathbf{S}	0	0	
41	DO	BS 103	770	486	142	141	1	0	0	

• Molecule 42 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
42	AT	94	Total 722	C 463	N 130	O 129	0	0



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Mol	Chain	Residues		Ato	ms	AltConf	Trace	
42	BT	94	Total 722	C 463	N 130	O 129	0	0

• Molecule 43 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
43	AU	82	Total 622	C 385	N 122	0 115	0	0
43	BU	82	Total 622	$\begin{array}{c} \mathrm{C} \\ 385 \end{array}$	N 122	0 115	0	0

• Molecule 44 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues		Aton	ns	AltConf	Trace		
44	AV	58	Total	С	Ν	0	0	0	
44 A	ΛV	- 10	445	277	96	72	0	0	
4.4	BV	59	Total	С	Ν	0	0	0	
44		- 50	445	277	96	72	0	0	

• Molecule 45 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
45	AW	67	Total 541	C 333	N 102	O 106	0	0
45	BW	67	Total 541	C 333	N 102	O 106	0	0

• Molecule 46 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues		Aton	ns	AltConf	Trace	
46	AX	58	Total 449	C 280	N 85	O 84	0	0
46	BX	58	Total 449	C 280	N 85	O 84	0	0

• Molecule 47 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	۸V	50	Total	С	Ν	Ο	S	0	0
		370	225	68	76	1	0	0	
47	$_{\rm PV}$	50	Total	С	Ν	Ο	S	0	0
41	DI	- 59	370	225	68	76	1	0	0



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

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
19	17	18	Total	С	Ν	Ο	\mathbf{S}	0	0
40 AZ	40	360	222	77	59	2	0	0	
18	B7	18	Total	С	Ν	Ο	S	0	0
40		40	360	222	77	59	2		U

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Δ.1	47	Total	С	Ν	0	S	0	0
49 A1	41	390	238	78	70	4	0	0	
40	R1	47	Total	С	Ν	Ο	S	0	0
49	DI	41	390	238	78	70	4	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace	
50	A2	43	Total 367	C 225	N 89	O 52	S 1	0	0
50	B2	43	Total 367	C 225	N 89	O 52	S 1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace	
51 A3	Λ 2	64	Total	С	Ν	Ο	S	0	0
	AJ		521	324	113	82	2		
51 B3	D 3	3 64	Total	С	Ν	Ο	S	0	0
	Do		521	324	113	82	2		0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	A4	37	Total	С	Ν	0	S	0	0
			295	186	60	44	5		
52	B4	4 37	Total	С	Ν	Ο	\mathbf{S}	0	0
			295	186	60	44	5		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















• Molecule 4: 30S ribosomal protein S4





• Molecule 6: 30S rib	posomal protein S6				
	59%				
Chain Bf:		99%			
•• •••••	**** *** ***		••••••	• •• • • • ••	<u>** **</u> *
M1 R2 N13 114 E15 E15 E16 E16 D17 A18 K19 K20 K20	L22 V23 E24 F26 F26 G28 C28 C28 L30 A31 T32	E33 G34 A35 E36 V37 L38 E39	A40 K41 D42 W43 W43 K45 K45 R46 R46 L48 L48 A49 Y50	E51 152 NN53 N54 F59 R64 V65 K66 S67	D68 N69 N70 A72 E75
** *** ***					
R78 L79 182 833 833 833 833 833 833 833 833 833 8					
• Molecule 7: 30S rib	posomal protein S7				
	68%				
Chain Ag:		100%			
11 13 13 13 14 11 11 11 11 11 11 11 11 11 11 11 11	14 15 16 17 17 20 20 22 22 23 23	255 448 49 50 51 52	53 554 555 55 55 56 61 61 61	63 64 65 66 66 66 66 71 77 77	74 775 776 778 778 778 80 81 81 83
Y CONTREDU	T T T T T T T T T T T T T T T T T T T		носночору		
**** *****	• • •• ••••	**** *	* ***** **	• ••••• •	•• ••
N84 Y85 Q86 Q86 P88 V87 P88 V89 C90 P93 P93 F93 P93	R96 T97 W103 W103 N106 T108 R109 R109 R1109 R1110 R11110	L120 A121 N122 E123 E123 L125	 b126 b126 b128 <lib128< li=""> b128<td>K137 K137 E139 E139 D140 T141 H142 H142 K143 M144 A145 E146</td><td>A147 N148 F151 A152 A152</td></lib128<>	K137 K137 E139 E139 D140 T141 H142 H142 K143 M144 A145 E146	A147 N148 F151 A152 A152
• Moleculo 7: 208 rih	ocomal protain \$7				
• Molecule 7. 505 III.					
Chain Bg:	0070	100%			
	4' 'n' n' 'n' n' n' n' n' n' n' n' n' n'				
M 66 86 86 86 87 87 87 87 87 87 87 87 87 87 87 87 87			RE GE DE DE LE E C F F	Ec Ec P; V; V;	A 77 77 77 7 7 7 7 7 7 7 7 7 7 7 7 7 7
•••• •••••	•• • •• ••••	*****	• ••••• ••	• • • • • • •	•• ••
N84 Y85 Q86 Q86 P88 V87 V89 K92 P93 P93 F894	R96 T97 W103 W106 N106 Y107 A108 R109 L1110 R111 C112	L120 A121 N122 E123 L124 L125	D126 A127 A128 N129 N130 T131 G132 G133 A134 V135 V135	K137 K137 E139 E139 D140 T141 H142 K143 K143 M144 A145 E146	A147 N148 F151 A152 A152
. Malaa la 0, 200 °l					
• Molecule 8: 305 rfb	51%				
Chain Ah:	51/6	98%		 .	
2 2 1 18 2 2 1 2 2 2 2 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	2 2 7 2 3 3 3 4 5 5 3 3 4 5 5 5 4 5 5 5 5 5 5 5	42 44 44 50 51 51	6 8 9 9 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7	70 71 73 73 75 76 77 76 77 77 77 77	88 88 88 88 80 88 88 88 88 88 88 88 88 88 88 88 88 88
	ча на жи на к				
*****	* * **** *	••••			
S92 E93 M94 P95 K96 K96 G100 C100 C100 C1002 C1003	E110 E117 E117 A118 R119 K120 K120 K120 R121 N122	1128 A129 Y130 V131 W132			
• Molecule & 308 rib	osomal protoin S8				
- molecule 0. 505 IIt	51%				
Chain Bh:		98%		.	









• Molecule 11: 30S ribosomal protein S11



 \bullet Molecule 11: 30S ribosomal protein S11





• Molecule 12: 30S ribosomal protein S12



 \bullet Molecule 13: 30S ribosomal protein S13





• Molecule 1	16: 30S ribosomal protein S16	
Chain Ap:	42% 98%	
A2 R9 D30 G31 R32 133	134 E35 E35 C336 C338 C338 C338 C338 C338 C338 C338	E36 Q87 K88 K89 A90
• Molecule 1	16: 30S ribosomal protein S16	
Chain Bp:	42% 98%	•
A2 R9 G31 S32	I34 E35 G36 G36 C38 C38 C38 C38 C38 C38 C38 C38 C38 C49 C45 C49 C45 C49 C45 C54 C54 C55 C55 C55 C55 C55 C55 C55	E86 Q87 K89 A90
• Molecule 1	17: 30S ribosomal protein S17	
Chain Aq:	52% 100%	•
N5 D6 V9 Y10 V11 G12	K13 V14 V15 S16 M19 K18 M19 K18 K27 F28 F28 F33 F33 K31 F28 K33 K34 K34 K34 K34 K33 K34 K34 K33 K33	E79 180 V81 E82 E82 E83 S84
• Molecule 1	17: 30S ribosomal protein S17	
Chain Bq:	54%	•
N5 0 D6 0 V9 V9 V11 0 V11 0 C12 0	K13 V14 V15 S16 S16 M19 M19 W27 K18 W27 W27 W132 W31 M132 W33 W34 W31 M132 W33 W34 W41 W42 W41 W42 M33 W33 W33 W33 W33 W33 W33 W33 W33 W33	E79 180 V81 E82 E83 S84
• Molecule 1	18: 30S ribosomal protein S18	
Chain Ar:	59% 98% •	i de la compañía de l
T24 H25 126 D27 Y28 K29 K29	T31 E32 L33 F35 F35 F37 F35 F35 E40 F45 F46 F46 F46 F46 F46 F46 F46 F46 F47 F56 F48 F47 F56 F48 F47 F66 F47 F47 F47 F47 F47 F47 F47 F47 F47 F47	
• Molecule 1	18: 30S ribosomal protein S18	
Chain Br:	59% 98% •	I

T24 H25 126 126 27 Y28 Y28 Y28 Y28 Y29	131 132 133 134 138 138 138 138 138 138 138 138 138 138 138 138 138 138 138 138 138 138 138 138 138 138 138 138 138 138 139 138 141 141 142 144 145 145 145 150 151 152 153 154 155 155 156 157 157 158 159 150 150 151 152 152 152 153 154 155 156 157 157 158 </td <td></td>	
• Molecule 1	19: 30S ribosomal protein S19	
Chain As:	99%	1



Chain Av:	82%	•	15%	
• Molecule 22: Ribo	some hibernation promoti 57%	on factor		
T4 V5 V6 K7 K8 K8 N9 E10 E112 E113 D14	L115 R117 F19 F19 K20 S22 S22 S24 K25 S26 S26 S26 S26 S26 S26 S26 S26 S26 S26	q30 E31 V32 V32 R33 R33 F37 F37 F37 F37 F39 F39 F39 F39 F41	V43 K44 R45 K46 K47 K47 A51 A51 A52 R53	K54 R55
Chain Bu:	100%		••••	••
• Molecule 21: 30S 1	ribosomal protein S21 94%			
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	Luca R17 R17 R17 R18 R17 R18 R28 S28 S28 S28 S28 S28 S28 S28 S	Q 20 E 31 V 32 V 32 V 32 F 33 F 33 F 33 F 33 F 34 F 34 F 34 F 34	V 45 K 46 K 46 K 47 K 47 K 47 K 47 K 47 K 47 K 45 Z 451	K54 R55
••••••		•••••	••••	••
Chain Au:	94% 100%			
• Molecule 21: 30S 1	ribosomal protein S21			
A2 14 K5 K5 A7 A7 R10 K12 K12 K12 T13	T14 E15 ← E15 ← R20 ← R25 ← R25 ← M41 ← M42 ← A3 ← A3 ← C58 ← A60 ← A60 ←	A61 462 863 863 868 868 972 477 77 77 881 881		
Chain Bt:	99%		·	
• Molecule 20: 30S 1	ibosomal protein S20 33%			
A2 N3 14 K5 K6 A7 A7 18 K9 K12 K12 K12	T14 E15 R20 R20 R20 R26 R44 R41 R44 R43 R43 R59 R58 R59 R58 R59 R58	461 662 863 863 868 868 868 872 977 777 777 777 881		
•••••••••	• • • • • • •			
Chain At:	33%			
• Molecule 20: 30S 1	ibosomal protein S20			
84 77 78 138 119 119 119 122 1220	225 225 227 227 228 229 229 259 447 141 141 141 141 141 141 141 141 141	2664 280 183 183 481 481		
Chain Bs:	99%		·	
• Molecule 19: 30S i	ibosomal protein S19			



























• Molecule 25: 50S ribosomal protein L2





• Molecule 26: 50S ribosomal protein L3



• Molecule 26: 50S ribosomal protein L3





• Molecule 27: 50S ribosomal protein L4





• Molecule 29: 50S ribosomal protein L6 55% Chain AG: 99% Q4 E4 E4 N4 N4 T4 E T5 E51 P55 S56 D57 D57 S58 S58 K59 I8 I9 D10 11: 11: P1: G2 H2 V2 T2 V113 E114 T115 K116 K116 A117 E118 E118 E118 N120 A96 Q97 M98 Q99 G10 L87 E88 L89 V90 C91 C91 V92 V92 C93 K10 • Molecule 29: 50S ribosomal protein L6 55% Chain BG: 99% T46 150 E51 18 19 10 11 11: 11: 11: 11: A96 Q97 M98 Q99 G10 L87 E88 V9C C91 C91 C91 C91 C93 • Molecule 30: 50S ribosomal protein L13 27% Chain AH: 99% E9 S1(0 N11 112 E13 T7 D7 K7 • Molecule 30: 50S ribosomal protein L13 27% Chain BH: 99% E9 S10 N11 E12 E13 A60 S61 K62 I63 E64 • Molecule 31: 50S ribosomal protein L14 64% Chain AI: 97% L114 V115 S116 S116 A115 P119 E120 D89 D9C K91 G92 P93 R94 C95 C95

• Molecule 31: 50S ribosomal protein L14






• Molecule 34: 50S ribosomal protein L17







• Molecule 39: 50S ribosomal protein L22



41% Chain BQ:	99%	
M1 E2 R8 T9 T10 T10 T12 T12 T24 T24 T24 T24 T24 T24 T24 T24 T24 T2	133 136 136 136 136 136 139 140 140 141 147 147 147 147 147 146 163 163 163 163	V71 V71 P80 F81 F82 F85 F85 F85 F85 F85 F85 F85 F85 F85 F85
• Molecule 40: 50S ribosomal protein	L23	
31%		
Chain AR:	98% •	
E2 A3 E18 A21 E22 E23 E24 B23 E24 C23 C23 C23 C23 C23 C23 C25 C22 C22 C22 C22 C22 C22 C22 C22 C22	K62 R64 M65 C66 C66 C66 C70 C71 C83 C71 C83 C85 C83 C85 C85 C85 C85 C85 C85 C85 C85 C85 C85	
• Molecule 40: 50S ribosomal protein	L23	
31%		
Chain BR:	98% •	•
E2 A3 A3 E14 E18 E22 E23 E24 E24 E24 E24 E24 E24 K49 K49 K49 K49 K49 K49 K49 K49 K49 K4	K62 R64 R64 R67 C66 C66 C66 C66 C66 C66 C66 C65 C66 C65 C66 C66	
• Molecule 41: 50S ribosomal protein	L24	
52%		
Chain AS:	99% •	
H2 G6 D7 D16 K17 K17 C18 K17 C18 K17 C18 K12 C21 K22 C21 K22 C21 K22 C21 K22 C21 K22 C21 K22 C21 K22 C21 K22 C21 K22 C21 K22 C21 K22 C21 K22 C21 K22 C21 K22 C21 K22 C21 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C22 K22 C2 K22 C2 K22 C2 K22 C2 K22 C2 K22 C2 K22 C2 K22 C2 K22 C2 K22 C2 K22 C2 K22 C2 K22 C2 K22 C2 K22 C2 K22 C2 K22 C2 K22 C2 K22 C2 K22 C2 C2 C2 K2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2	N39 M41 K42 K43 K43 K45 P47 P45 P45 P62 E53 E53 E53 E53 E53 E53 E53 F52 F52 F53 F53 F53 F53 F53 F53 F53 F53 F53 F53	L71 D72 P73 K74 T75 E77 E77 E85 V86 V86 C88 C88 C88 C88 C88 C88
K90 897 698 E100 K102 S103 N104		
• Molecule 41: 50S ribosomal protein	L24	
52%		
Chain BS:	99%	
H2 G6 D7 D16 K119 K119 C118 K119 C118 K119 C118 K120 K22 K22 K22 K230 K37 K30 K37 K30 K37 K30 K37 K30 K37 K38 K38 K38 K38 K38 K38 K38 K38 K38 K38	N39 M41 K42 K43 K46 F47 C46 Q49 C50 P52 P52 P52 P52 P52 P52 P52 P52 P52 P52	L71 D72 P73 K74 K74 E77 E77 F85 F85 F85 C88 K89
K90 897 698 E100 K102 S103		
• Molecule 42: 50S ribosomal protein	L25	
Chain ATL		
Unalli A1:	99% ·	
	PROTEIN DATA BANK	

A2 K5 K5 K5 K5 K5 R9 R1 R1 R1 R1 R1 K19 K19	q20 L21 K22 S24 S24 C25 K26 V27 V27 Y34 K37 K37 K37 K37 K37 K38 K38 K38 V39 V41 K42 V41 V41	 V46 E47 F48 K50 K51 K53 K55 K56 K57 K57 K57 K57 K56 K57 K57 K57 K57 K57 K57 K57 K57 K57 K58 K58 K68 K68
K71 V72 V72 V73 V74 V75 V77 V77 V77 V77 V77 V77 V77 V78 V78 V78 V78 V78 V78 V78 V84 V84 V84 V84 V84 V84 V84 V84 V84 V84 V84 V84 V84 V74 V74 V75 V76 V76 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77 V77	035 186 A93 N95	
• Molecule 42: 50S ribo	somal protein L25	
Chain BT:	76% 99%	
A2 S3 K5 K5 S6 S6 17 R9 R9 R1 R1 R12 K12 K19	q20 L21 R22 K23 S24 G25 C25 K26 V27 V27 V34 C35 C35 C35 C35 C35 C35 C35 C35 C35 C35	 446 F48 F48 F48 F49 K50 K50 K53 F54 K55 G56 G59 G59 G59 G59 G56 G64 G65 G64 G64
K71 V72 M73 M74 A75 A75 F79 F79 F79 F81 K83 K83 K83 K83		
• Molecule 43: 50S ribo	somal protein L27	
Chain AU:	95%	5%
K12 K13 G14 V15 S16 S17 T18 K12 C21 K22 C21 K22 C21 K22 C21 K22 C21 K22 C21 K22 C21 K22 C21 K22 K13 K13 K13 K13 K13 K13 K13 K13 K13 K13	R61 N90 A91 A93 A93	
• Molecule 43: 50S ribo	somal protein L27	
Chain BU:	95%	5%
K12 K13 C14 C14 C14 S15 S16 S17 T18 K19 M20 M20 R22 R22 R22 R22 R22 R22 R22 R22 R22 R	N61 N75 N90 A91 A93 A93	
• Molecule 44: 50S ribo	somal protein L28	
Chain AV:	59% 98%	.
K3 Q4 C5 C5 F6 V7 C1 C5 C5 C1 C5 C1 C5 C1 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5	H20 T25 K26 R27 R27 R27 R37 L38 L39 C40 C41 C42 C42 C42 C42 C42 C42 C42 C42 C42 C42	
• Molecule 44: 50S ribo	somal protein L28	
Chain BV:	98%	
K3 Q4 C5 C5 C5 F6 K1 K1 K11 K11 K12 S13 S13	H20 125 K26 K27 K27 R37 R37 R37 R37 R28 R28 R46 K43 F44 K45 K45 K45 K46 K46 K46 K46	

 \bullet Molecule 45: 50S ribosomal protein L29



	48%	_	
Chain AW:		100%	
• •• •••••	•••••	• •• ••••	
K2 A3 K4 E5 E5 I6 R7 D8 L9 T10 T11	812 E13 E15 E15 E16 E16 Q17 T18 X19 X19 X19 X19 X19 C35 C35 C35 C35 C35 C35 C35 C35 C35 C35	R42 A57 E59 E59 R60 E63 E63 E63 E63 C66 K66 K66 K66 N68 N68	
• Molecule 45: 5	0S ribosomal protein L29		
	48%	_	
Chain BW:		100%	
K2 A3 K4 E5 E5 R7 C8 C9 D8 C9 C9 T10	S12 E13 E14 E15 E15 Q17 118 K19 S20 S20 C35 G35 Q36 Q36 Q36	R42 A57 R56 R56 R60 E61 E61 E63 E63 E63 C66 K66 A67 N66	
• Molecule 46: 5	0S ribosomal protein L30		
	62%		
Chain AX:		100%	
A2 K3 L4 L8 R10 S11 V12	E.17 118 019 R.20 K.21 F.22 K.23 E.24 K.28 K.29 K.28 K.29 K.28 K.29 K.30 K.30 K.31 K.30 K.30 K.30 K.30 K.31 K.31 K.31 K.31 K.31 K.31 K.31 K.31	V35 V35 V37 E38 D39 D39 H47 K49 K51 H52 K51 H52 C53 K51 H52 K51 E53 V56 E57 E57 K59	
• Molecule 46: 5	0S ribosomal protein L30		
	62%		
Chain BA:		100%	
		x x x x x x x x x x x x x x x x x x x	
A2 K3 L4 L8 T5 R1 R1 S1 S1 V1	E1 0 0 11 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	и 3 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	
• Molecule 47: 5	0S ribosomal protein L31	type B	
Chain AY:	90%	100%	
M1 K2 G4 15 F7 F8 K9 K9	411 713 113 113 113 113 113 113 113 113 1	S27 T28 K29 K29 S31 S31 S31 S31 S33 S32 S33 S33 S33 S33 S33 S33 S34 V45 V45 V45 V45 V45 V45 V45 V45 V45 V4	ьчо D49 I50 S51 S51 H55 F57 F57 Y58 T59 T59
• Molecule 47: 5	0S ribosomal protein L31	type B	
Chain BY:	90%	100%	
M1 K2 Q3 G4 F7 F7 F9 K9	0111 113 113 113 113 113 114 114 114 114	227 128 128 130 1331 5331 5331 833 833 833 833 833 833 833 833 840 840 840 840 840 842 842 842 842 842 842 842 842 842 842	Liao D49 150 S51 S52 S52 F55 F55 758 T59
• Molecule 48: 5	0S ribosomal protein L32		
Chain AZ:	40%	100%	
CHUIH 112.		10070	
A2 R12 F20 K21 I22 S23 S23 Y24 P25	P31 N32 C33 C33 C33 C33 C33 C33 C33 C33 C34 C43 C43		
		PROTEIN DATA BANK	

• Molecule 48: 50S ribosomal protein L32







 \bullet Molecule 52: 50S ribosomal protein L36







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12570	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	2.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.059	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.023	Depositor
Map size (Å)	642.0, 642.0, 642.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.605, 1.605, 1.605	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

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

Mol Chain		Bo	ond lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	Aa	0.38	0/36913	0.95	101/57564~(0.2%)	
1	Ba	0.38	0/36913	0.95	102/57564~(0.2%)	
2	Ab	0.26	0/1840	0.53	1/2470~(0.0%)	
2	Bb	0.26	0/1840	0.53	1/2470~(0.0%)	
3	Ac	0.27	0/1523	0.59	0/2062	
3	Bc	0.27	0/1523	0.59	0/2062	
4	Ad	0.28	0/1526	0.62	1/2063~(0.0%)	
4	Bd	0.28	0/1526	0.62	1/2063~(0.0%)	
5	Ae	0.28	0/1159	0.59	0/1566	
5	Be	0.28	0/1159	0.59	0/1566	
6	Af	0.30	0/789	0.60	1/1060~(0.1%)	
6	Bf	0.30	0/789	0.60	1/1060~(0.1%)	
7	Ag	0.26	0/1176	0.54	0/1588	
7	Bg	0.26	0/1176	0.54	0/1588	
8	Ah	0.31	0/1038	0.63	0/1395	
8	Bh	0.31	0/1038	0.63	0/1395	
9	Ai	0.27	0/937	0.67	1/1269~(0.1%)	
9	Bi	0.27	0/937	0.67	1/1269~(0.1%)	
10	Aj	0.27	0/764	0.56	0/1034	
10	Bj	0.27	0/764	0.56	0/1034	
11	Ak	0.29	0/824	0.59	0/1119	
11	Bk	0.29	0/824	0.59	0/1119	
12	Al	0.30	0/1054	0.63	1/1415~(0.1%)	
12	Bl	0.30	0/1054	0.63	1/1415~(0.1%)	
13	Am	0.26	0/732	0.56	0/991	
13	Bm	0.26	0/732	0.56	0/991	
14	An	0.32	0/497	0.63	0/662	
14	Bn	0.32	0/497	0.63	0/662	
15	Ao	0.26	0/732	0.53	0/979	
15	Bo	0.26	0/732	0.53	0/979	
16	Ap	0.33	0/705	0.57	0/952	
16	Bp	0.33	0/705	0.57	0/952	
17	Aq	0.32	0/629	0.58	0/849	
17	Bq	0.32	0/629	0.58	0/849	



		Bo	ond lengths	Bond angles		
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
18	Ar	0.28	0/453	0.65	1/604~(0.2%)	
18	Br	0.28	0/453	0.65	1/604~(0.2%)	
19	As	0.31	0/654	0.58	0/879	
19	Bs	0.31	0/654	0.58	0/879	
20	At	0.23	0/591	0.50	0/793	
20	Bt	0.23	0/591	0.50	0/793	
21	Au	0.27	0/403	0.51	0/535	
21	Bu	0.27	0/403	0.51	0/535	
22	Av	0.49	0/1350	0.81	2/1812~(0.1%)	
22	Bv	0.49	0/1350	0.81	2/1812~(0.1%)	
23	AA	0.74	3/69738~(0.0%)	1.02	207/108747~(0.2%)	
23	BA	0.74	3/69738~(0.0%)	1.02	208/108747~(0.2%)	
24	AB	0.61	0/2732	1.16	21/4253~(0.5%)	
24	BB	0.61	0/2732	1.16	21/4253~(0.5%)	
25	AC	0.48	0/2129	0.67	3/2858~(0.1%)	
25	BC	0.48	0/2129	0.67	3/2858~(0.1%)	
26	AD	0.49	0/1651	0.66	0/2215	
26	BD	0.49	0/1651	0.66	0/2215	
27	AE	0.47	0/1595	0.66	0/2154	
27	BE	0.47	0/1595	0.66	0/2154	
28	AF	0.31	0/1339	0.63	0/1805	
28	BF	0.32	0/1339	0.63	0/1805	
29	AG	0.35	0/1281	0.58	0/1736	
29	BG	0.35	0/1281	0.58	0/1736	
30	AH	0.48	0/1165	0.65	0/1570	
30	BH	0.48	0/1165	0.65	0/1570	
31	AI	0.47	0/925	0.73	3/1242~(0.2%)	
31	BI	0.47	0/925	0.73	3/1242~(0.2%)	
32	AJ	0.46	0/1100	0.71	2/1467~(0.1%)	
32	BJ	0.45	0/1100	0.71	$2/1467 \ (0.1\%)$	
33	AK	0.46	0/1095	0.61	0/1472	
33	BK	0.46	0/1095	0.61	0/1472	
34	AL	0.43	0/936	0.71	0/1253	
34	BL	0.43	0/936	0.71	0/1253	
35	AM	0.43	0/900	0.69	3/1205 (0.2%)	
35	BM	0.43	0/900	0.69	2/1205 (0.2%)	
36	AN	0.44	0/901	0.65	1/1209 (0.1%)	
36	BN	0.44	0/901	0.65	1/1209 (0.1%)	
37	AO	0.52	0/954	0.64	0/1264	
37	BO	0.52	0/954	0.64	0/1264	
38	AP	0.47	0/800	0.67	0/1070	
38	BP	0.47	0/800	0.67	0/1070	
39	AQ	0.45	0/862	0.70	0/1161	



Mal	Chain	Bo	ond lengths]	Bond angles
10101	Ullaill	RMSZ	# Z > 5	RMSZ	# Z > 5
39	BQ	0.45	0/862	0.70	0/1161
40	AR	0.43	0/723	0.63	0/966
40	BR	0.43	0/723	0.63	0/966
41	AS	0.39	0/779	0.67	0/1043
41	BS	0.39	0/779	0.67	0/1043
42	AT	0.37	0/730	0.66	1/981~(0.1%)
42	BT	0.37	0/730	0.66	1/981~(0.1%)
43	AU	0.55	0/628	0.68	1/833~(0.1%)
43	BU	0.55	0/628	0.68	1/833~(0.1%)
44	AV	0.38	0/451	0.66	0/603
44	BV	0.38	0/451	0.66	0/603
45	AW	0.39	0/542	0.69	0/722
45	BW	0.39	0/542	0.69	0/722
46	AX	0.40	0/451	0.61	0/606
46	BX	0.40	0/451	0.61	0/606
47	AY	0.25	0/378	0.53	0/521
47	BY	0.25	0/378	0.53	0/521
48	AZ	0.43	0/366	0.65	0/489
48	ΒZ	0.43	0/366	0.65	0/489
49	A1	0.34	0/395	0.60	0/530
49	B1	0.34	0/395	0.60	0/530
50	A2	0.48	0/371	0.67	0/484
50	B2	0.47	0/371	0.67	0/484
51	A3	0.40	0/526	0.62	0/690
51	B3	0.40	0/526	0.61	0/690
52	A4	0.53	0/298	0.63	0/392
52	B4	0.52	0/298	0.63	0/392
All	All	0.58	$6/3\overline{06060}\ (0.0\%)$	0.92	703/458404~(0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	Ae	0	1
5	Be	0	1
9	Ai	0	1
9	Bi	0	1
12	Al	0	1
12	Bl	0	1
19	As	0	1



Mol	Chain	#Chirality outliers	#Planarity outliers
19	Bs	0	1
20	At	0	1
20	Bt	0	1
26	AD	0	1
26	BD	0	1
38	AP	0	1
38	BP	0	1
All	All	0	14

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BA	1065	А	N9-C4	-5.38	1.34	1.37
23	AA	1584	U	C1'-N1	5.31	1.56	1.48
23	BA	1584	U	C1'-N1	5.31	1.56	1.48
23	AA	1065	А	N9-C4	-5.26	1.34	1.37
23	BA	1186	А	N9-C4	-5.21	1.34	1.37
23	AA	1186	А	N9-C4	-5.02	1.34	1.37

All (703) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
24	BB	87	С	N1-C2-O2	12.71	126.53	118.90
24	AB	87	С	N1-C2-O2	12.65	126.49	118.90
24	AB	87	С	C2-N1-C1'	12.14	132.15	118.80
24	BB	87	С	C2-N1-C1'	12.08	132.08	118.80
23	AA	576	U	C2-N1-C1'	12.02	132.13	117.70
23	BA	576	U	C2-N1-C1'	11.98	132.07	117.70
1	Aa	745	U	OP1-P-O3'	-11.41	80.09	105.20
1	Ba	745	U	OP1-P-O3'	-11.40	80.12	105.20
23	AA	2150	А	N7-C8-N9	10.86	119.23	113.80
23	BA	2150	А	N7-C8-N9	10.83	119.22	113.80
23	BA	576	U	N1-C2-O2	10.59	130.21	122.80
24	AB	111	С	N1-C2-O2	10.59	125.25	118.90
24	BB	111	С	N1-C2-O2	10.59	125.25	118.90
24	AB	87	С	N3-C2-O2	-10.55	114.52	121.90
23	AA	576	U	N1-C2-O2	10.55	130.18	122.80
23	BA	1179	С	N1-C2-O2	10.49	125.19	118.90
24	BB	87	С	N3-C2-O2	-10.47	114.57	121.90
23	AA	1179	C	N1-C2-O2	10.42	125.15	118.90
23	BA	576	U	N3-C2-O2	-9.97	115.22	122.20
23	AA	576	U	N3-C2-O2	-9.96	115.23	122.20



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
23	BA	2150	А	C5-N7-C8	9.83	108.81	103.90
23	AA	2150	А	C5-N7-C8	9.79	108.80	103.90
23	AA	1994	С	N1-C2-O2	9.75	124.75	118.90
23	BA	1994	С	N1-C2-O2	9.72	124.73	118.90
23	BA	1994	С	C2-N1-C1'	9.61	129.37	118.80
23	AA	1994	С	C2-N1-C1'	9.60	129.37	118.80
23	AA	1932	С	N1-C2-O2	9.50	124.60	118.90
23	BA	1932	С	N1-C2-O2	9.41	124.55	118.90
23	BA	1932	С	C2-N1-C1'	9.39	129.13	118.80
23	AA	1932	С	C2-N1-C1'	9.36	129.10	118.80
24	BB	87	С	C6-N1-C1'	-9.05	109.94	120.80
24	AB	87	С	C6-N1-C1'	-9.04	109.95	120.80
23	AA	1179	С	N3-C2-O2	-8.82	115.72	121.90
23	BA	1179	С	N3-C2-O2	-8.78	115.75	121.90
23	AA	1179	С	C2-N1-C1'	8.75	128.42	118.80
24	AB	111	С	N3-C2-O2	-8.74	115.78	121.90
23	BA	1179	С	C2-N1-C1'	8.71	128.38	118.80
24	BB	111	С	N3-C2-O2	-8.69	115.82	121.90
24	BB	111	С	C2-N1-C1'	8.63	128.29	118.80
23	AA	593	U	C2-N1-C1'	8.61	128.03	117.70
24	AB	111	С	C2-N1-C1'	8.60	128.26	118.80
23	BA	593	U	C2-N1-C1'	8.56	127.97	117.70
24	BB	108	U	N3-C2-O2	-8.44	116.29	122.20
24	AB	108	U	N3-C2-O2	-8.42	116.31	122.20
23	AA	439	U	C2-N1-C1'	8.37	127.74	117.70
23	AA	576	U	C6-N1-C1'	-8.35	109.50	121.20
23	BA	576	U	C6-N1-C1'	-8.33	109.53	121.20
23	AA	1894	G	C4-N9-C1'	8.33	137.33	126.50
23	BA	1894	G	C4-N9-C1'	8.33	137.33	126.50
23	BA	439	U	C2-N1-C1'	8.32	127.69	117.70
23	AA	1378	U	N3-C2-O2	-8.30	116.39	122.20
9	Bi	66	LEU	CA-CB-CG	8.29	134.38	115.30
9	Ai	66	LEU	CA-CB-CG	8.29	134.37	115.30
23	BA	1378	U	N3-C2-O2	-8.22	116.45	122.20
23	BA	1804	U	C2-N1-C1'	8.19	127.53	117.70
1	Aa	55	C	N1-C2-O2	8.13	123.78	118.90
23	AA	1804	U	C2-N1-C1'	8.12	$1\overline{27.44}$	117.70
1	Ba	55	C	N1-C2-O2	8.10	$123.7\overline{6}$	118.90
23	AA	1378	U	N1-C2-O2	8.08	128.46	122.80
23	BA	1378	U	N1-C2-O2	8.07	128.45	122.80
1	Aa	99	U	$C2-N1-\overline{C1'}$	8.07	$127.3\overline{8}$	117.70
24	BB	108	U	C2-N1-C1'	8.06	127.37	117.70



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Ba	99	U	C2-N1-C1'	8.05	127.37	117.70
24	BB	100	U	C2-N1-C1'	8.05	127.36	117.70
24	AB	108	U	C2-N1-C1'	8.04	127.35	117.70
1	Aa	599	U	C2-N1-C1'	8.03	127.34	117.70
1	Ba	599	U	C2-N1-C1'	8.03	127.34	117.70
1	Ba	55	С	C2-N1-C1'	8.02	127.62	118.80
23	AA	759	U	C2-N1-C1'	8.02	127.32	117.70
23	BA	759	U	N1-C2-O2	8.02	128.41	122.80
23	BA	1994	С	N3-C2-O2	-8.00	116.30	121.90
24	AB	100	U	C2-N1-C1'	8.00	127.29	117.70
23	BA	759	U	C2-N1-C1'	8.00	127.29	117.70
23	AA	759	U	N1-C2-O2	7.98	128.38	122.80
1	Aa	55	С	C2-N1-C1'	7.97	127.57	118.80
23	AA	1994	С	N3-C2-O2	-7.97	116.32	121.90
1	Ba	1187	G	C4-N9-C1'	7.94	136.82	126.50
1	Aa	1187	G	C4-N9-C1'	7.92	136.80	126.50
23	BA	439	U	N3-C2-O2	-7.88	116.68	122.20
23	AA	439	U	N3-C2-O2	-7.87	116.69	122.20
23	AA	1227	U	N3-C2-O2	-7.84	116.71	122.20
23	AA	439	U	N1-C2-O2	7.84	128.29	122.80
23	BA	439	U	N1-C2-O2	7.84	128.29	122.80
1	Ba	745	U	OP2-P-O3'	-7.79	88.07	105.20
1	Aa	745	U	OP2-P-O3'	-7.78	88.09	105.20
23	BA	1227	U	N3-C2-O2	-7.75	116.78	122.20
23	BA	2370	U	N3-C2-O2	-7.73	116.79	122.20
23	BA	882	С	C2-N1-C1'	7.70	127.27	118.80
23	AA	2370	U	N3-C2-O2	-7.69	116.82	122.20
23	AA	882	С	C2-N1-C1'	7.68	127.25	118.80
23	AA	1378	U	C2-N1-C1'	7.63	126.86	117.70
23	AA	1932	С	N3-C2-O2	-7.63	116.56	121.90
23	BA	1378	U	C2-N1-C1'	7.62	126.84	117.70
24	AB	108	U	N1-C2-O2	7.59	128.12	122.80
24	BB	108	U	N1-C2-O2	7.59	128.11	122.80
31	AI	20	LEU	CA-CB-CG	7.56	132.69	115.30
31	BI	20	LEU	CA-CB-CG	7.55	132.66	115.30
23	AA	1894	G	C8-N9-C1'	-7.53	117.20	127.00
23	BA	1894	G	C8-N9-C1'	-7.53	117.20	127.00
23	BA	1932	С	N3-C2-O2	-7.50	116.65	121.90
1	Ba	1136	U	C2-N1-C1'	7.48	126.67	117.70
35	BM	31	LEU	CA-CB-CG	7.44	132.41	115.30
$\overline{35}$	AM	31	LEU	CA-CB-CG	7.42	132.37	115.30
1	Aa	1136	U	C2-N1-C1'	7.41	126.59	117.70



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
23	AA	1599	G	N3-C2-N2	-7.41	114.72	119.90
1	Ba	415	А	P-O3'-C3'	7.35	128.52	119.70
23	BA	1599	G	N3-C2-N2	-7.29	114.79	119.90
1	Aa	415	А	P-O3'-C3'	7.29	128.45	119.70
23	AA	1692	С	C2-N1-C1'	7.28	126.81	118.80
23	BA	1692	С	C2-N1-C1'	7.26	126.78	118.80
23	BA	1579	С	N1-C2-O2	7.22	123.23	118.90
1	Ba	902	С	C2-N1-C1'	7.17	126.69	118.80
23	AA	1579	С	N1-C2-O2	7.17	123.20	118.90
23	BA	1994	С	C6-N1-C1'	-7.16	112.21	120.80
23	AA	1597	U	N3-C2-O2	-7.14	117.20	122.20
1	Aa	835	U	C2-N1-C1'	7.13	126.26	117.70
23	AA	2223	С	N1-C2-O2	7.13	123.18	118.90
1	Aa	746	U	OP1-P-OP2	7.11	130.27	119.60
1	Aa	902	С	C2-N1-C1'	7.11	126.62	118.80
1	Ba	835	U	C2-N1-C1'	7.11	126.23	117.70
23	AA	1994	С	C6-N1-C1'	-7.10	112.28	120.80
23	BA	1932	С	C6-N1-C1'	-7.09	112.29	120.80
1	Ba	746	U	OP1-P-OP2	7.08	130.22	119.60
1	Ba	99	U	N1-C2-O2	7.08	127.75	122.80
1	Aa	99	U	N1-C2-O2	7.06	127.75	122.80
23	BA	1597	U	N3-C2-O2	-7.06	117.26	122.20
1	Ba	99	U	N3-C2-O2	-7.04	117.27	122.20
23	BA	2223	С	N1-C2-O2	7.04	123.12	118.90
23	AA	1932	С	C6-N1-C1'	-7.03	112.36	120.80
1	Aa	1187	G	N3-C4-N9	7.02	130.21	126.00
1	Aa	99	U	N3-C2-O2	-7.01	117.29	122.20
23	BA	759	U	N3-C2-O2	-7.00	117.30	122.20
1	Aa	460	А	P-O3'-C3'	6.99	128.09	119.70
23	BA	2261	G	P-O3'-C3'	-6.99	111.31	119.70
23	AA	1894	G	N3-C4-N9	6.97	130.18	126.00
23	BA	1894	G	N3-C4-N9	6.97	130.18	126.00
23	BA	2819	С	N1-C2-O2	6.97	123.08	118.90
1	Ba	1187	G	N3-C4-N9	6.94	130.16	126.00
23	AA	759	U	N3-C2-O2	-6.94	117.34	122.20
23	AA	2261	G	P-O3'-C3'	-6.94	111.38	119.70
1	Ba	460	А	P-O3'-C3'	6.93	128.01	119.70
23	AA	1214	C	N1-C2-O2	6.91	123.05	118.90
23	AA	1914	C	N1-C2-O2	6.89	123.03	118.90
23	BA	575	G	C4-N9-C1'	6.88	135.44	126.50
23	AA	575	G	C4-N9-C1'	6.85	135.41	126.50
23	BA	1914	С	N1-C2-O2	6.85	123.01	118.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
23	BA	2361	U	C2-N1-C1'	6.84	125.91	117.70
1	Aa	431	G	C4-N9-C1'	6.84	135.39	126.50
23	AA	1160	С	N1-C2-O2	6.84	123.00	118.90
1	Ba	431	G	C4-N9-C1'	6.84	135.39	126.50
1	Aa	424	G	C4-N9-C1'	6.84	135.39	126.50
1	Ba	424	G	C4-N9-C1'	6.84	135.39	126.50
22	Av	176	ARG	NE-CZ-NH1	6.83	123.72	120.30
22	Bv	176	ARG	NE-CZ-NH1	6.83	123.72	120.30
23	AA	2819	С	N1-C2-O2	6.82	122.99	118.90
23	BA	1160	С	N1-C2-O2	6.81	122.99	118.90
23	AA	2361	U	C2-N1-C1'	6.79	125.85	117.70
1	Aa	1187	G	N3-C4-C5	-6.76	125.22	128.60
1	Ba	1187	G	N3-C4-C5	-6.76	125.22	128.60
1	Aa	55	С	N3-C2-O2	-6.74	117.18	121.90
23	BA	1214	С	N1-C2-O2	6.74	122.94	118.90
1	Ba	55	С	N3-C2-O2	-6.71	117.20	121.90
1	Ba	431	G	N3-C4-N9	6.69	130.01	126.00
1	Aa	424	G	N3-C4-C5	-6.68	125.26	128.60
23	BA	1227	U	N1-C2-O2	6.65	127.45	122.80
23	AA	1227	U	N1-C2-O2	6.63	127.44	122.80
1	Ba	424	G	N3-C4-C5	-6.63	125.29	128.60
1	Aa	711	G	P-O3'-C3'	6.62	127.65	119.70
1	Aa	431	G	N3-C4-N9	6.60	129.96	126.00
1	Ba	711	G	P-O3'-C3'	6.60	127.62	119.70
1	Ba	451	U	P-O3'-C3'	6.59	127.61	119.70
1	Aa	1041	С	P-O3'-C3'	6.58	127.59	119.70
1	Aa	65	G	P-O3'-C3'	6.57	127.58	119.70
1	Aa	451	U	P-O3'-C3'	6.56	127.57	119.70
1	Ba	1041	С	P-O3'-C3'	6.55	127.56	119.70
1	Ba	65	G	P-O3'-C3'	6.54	127.55	119.70
23	BA	1597	U	N1-C2-O2	6.54	127.38	122.80
23	AA	1597	U	N1-C2-O2	6.53	127.37	122.80
1	Ba	1075	G	P-O3'-C3'	6.52	127.52	119.70
1	Ba	1187	G	C8-N9-C1'	-6.51	118.53	127.00
4	Ad	101	LEU	CA-CB-CG	6.51	130.28	115.30
1	Aa	1187	G	C8-N9-C1'	-6.51	118.54	127.00
4	Bd	101	LEU	CA-CB-CG	6.51	130.26	115.30
1	Aa	1075	G	P-O3'-C3'	6.50	127.50	119.70
1	Ba	$11\overline{36}$	U	N3-C2-O2	-6.49	117.66	122.20
1	Aa	1136	U	N3-C2-O2	-6.49	117.66	122.20
23	BA	2049	U	$C2-N1-\overline{C1'}$	$6.4\overline{8}$	$125.4\overline{7}$	117.70
1	Aa	835	U	N3-C2-O2	-6.47	117.67	122.20



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
23	AA	2049	U	C2-N1-C1'	6.46	125.46	117.70
1	Aa	336	С	C2-N1-C1'	6.46	125.91	118.80
1	Aa	315	U	C2-N1-C1'	6.45	125.44	117.70
1	Ba	336	С	C2-N1-C1'	6.45	125.89	118.80
23	BA	2699	U	N1-C2-O2	6.45	127.31	122.80
23	AA	2223	С	N3-C2-O2	-6.44	117.39	121.90
1	Ba	315	U	C2-N1-C1'	6.44	125.42	117.70
23	AA	575	G	N3-C4-N9	6.43	129.86	126.00
23	AA	1731	G	P-O3'-C3'	6.43	127.42	119.70
23	AA	268	А	P-O3'-C3'	6.43	127.42	119.70
23	BA	74	U	N1-C2-O2	6.42	127.30	122.80
23	BA	1213	С	N1-C2-O2	6.42	122.75	118.90
23	AA	2699	U	N1-C2-O2	6.41	127.29	122.80
1	Ba	431	G	N3-C4-C5	-6.41	125.39	128.60
23	BA	268	А	P-O3'-C3'	6.41	127.39	119.70
23	AA	1651	С	N1-C2-O2	6.40	122.74	118.90
23	BA	1651	С	N1-C2-O2	6.40	122.74	118.90
23	AA	74	U	N1-C2-O2	6.40	127.28	122.80
23	BA	1731	G	P-O3'-C3'	6.40	127.38	119.70
1	Ba	835	U	N3-C2-O2	-6.40	117.72	122.20
23	AA	1213	С	N1-C2-O2	6.39	122.73	118.90
23	AA	2450	U	P-O3'-C3'	6.39	127.36	119.70
23	BA	2450	U	P-O3'-C3'	6.39	127.36	119.70
24	BB	111	С	C6-N1-C1'	-6.38	113.14	120.80
23	BA	2223	С	N3-C2-O2	-6.38	117.43	121.90
1	Aa	1136	U	N1-C2-O2	6.38	127.27	122.80
23	BA	975	U	N1-C2-O2	6.37	127.26	122.80
23	AA	1992	С	C2-N1-C1'	6.36	125.80	118.80
23	BA	1552	U	N3-C2-O2	-6.36	117.75	122.20
24	AB	111	С	C6-N1-C1'	-6.35	113.18	120.80
23	BA	1992	С	C2-N1-C1'	6.35	125.78	118.80
23	AA	975	U	N1-C2-O2	6.34	127.24	122.80
23	AA	1804	U	C6-N1-C1'	-6.34	112.32	121.20
1	Ba	424	G	N3-C4-N9	6.34	129.80	126.00
23	BA	2262	G	O5'-P-OP1	-6.34	99.99	105.70
23	AA	1804	U	N3-C2-O2	-6.33	117.77	122.20
1	Ba	1136	U	N1-C2-O2	6.33	127.23	122.80
23	BA	1804	U	C6-N1-C1'	-6.33	112.33	121.20
1	Aa	424	G	N3-C4-N9	6.33	129.80	126.00
23	AA	1804	U	N1-C2-O2	6.32	127.23	122.80
23	BA	1804	U	N3-C2-O2	-6.32	117.77	122.20
23	AA	2747	U	C2-N1-C1'	6.32	125.28	117.70

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Ba	902	С	N3-C2-O2	-6.32	117.48	121.90
1	Aa	431	G	N3-C4-C5	-6.31	125.45	128.60
23	AA	2262	G	O5'-P-OP1	-6.29	100.03	105.70
23	BA	1692	С	N1-C2-O2	6.28	122.67	118.90
1	Aa	762	С	C2-N1-C1'	6.28	125.70	118.80
1	Ba	762	С	C2-N1-C1'	6.28	125.70	118.80
23	BA	2747	U	C2-N1-C1'	6.26	125.21	117.70
23	AA	988	С	N1-C2-O2	6.25	122.65	118.90
1	Aa	902	С	N3-C2-O2	-6.25	117.53	121.90
23	BA	575	G	N3-C4-N9	6.25	129.75	126.00
23	AA	1552	U	N3-C2-O2	-6.25	117.83	122.20
1	Ba	797	U	C2-N1-C1'	6.24	125.19	117.70
23	BA	862	С	N1-C2-O2	6.24	122.65	118.90
24	BB	94	С	N1-C2-O2	6.24	122.64	118.90
23	AA	1692	С	N1-C2-O2	6.24	122.64	118.90
23	BA	988	С	N1-C2-O2	6.23	122.64	118.90
1	Aa	902	С	N1-C2-O2	6.23	122.64	118.90
1	Aa	797	U	C2-N1-C1'	6.22	125.17	117.70
1	Aa	387	С	C2-N1-C1'	6.21	125.64	118.80
23	BA	1579	С	N3-C2-O2	-6.21	117.55	121.90
23	BA	184	С	C2-N1-C1'	6.21	125.63	118.80
23	AA	1227	U	C2-N1-C1'	6.20	125.14	117.70
1	Aa	1168	С	N1-C2-O2	6.20	122.62	118.90
23	AA	1579	С	N3-C2-O2	-6.19	117.56	121.90
23	AA	184	С	C2-N1-C1'	6.19	125.61	118.80
23	AA	862	С	N1-C2-O2	6.19	122.61	118.90
1	Ba	599	U	N1-C2-O2	6.19	127.13	122.80
1	Aa	599	U	N1-C2-O2	6.18	127.12	122.80
23	BA	1804	U	N1-C2-O2	6.17	127.12	122.80
23	BA	1953	U	C2-N1-C1'	6.17	125.11	117.70
23	AA	1953	U	C2-N1-C1'	6.17	125.11	117.70
24	AB	94	С	N1-C2-O2	6.17	122.60	118.90
23	BA	1227	U	C2-N1-C1'	6.17	125.11	117.70
23	AA	2845	G	N3-C2-N2	-6.17	115.58	119.90
1	Aa	835	U	N1-C2-O2	6.17	127.12	122.80
1	Ba	902	С	N1-C2-O2	6.17	122.60	118.90
23	AA	1914	С	N3-C2-O2	-6.16	117.59	121.90
1	Ba	387	C	C2-N1-C1'	6.16	125.58	118.80
1	Aa	1001	U	P-O3'-C3'	6.15	127.08	119.70
18	Ar	60	LEU	CA-CB-CG	6.15	129.45	115.30
1	Ba	835	U	N1-C2-O2	6.15	127.11	122.80
18	Br	60	LEU	CA-CB-CG	6.15	129.44	115.30



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Ba	502	С	C2-N1-C1'	6.15	125.56	118.80
23	AA	2845	G	N3-C4-N9	-6.15	122.31	126.00
1	Aa	524	U	C2-N1-C1'	6.14	125.07	117.70
1	Ba	1168	С	N1-C2-O2	6.13	122.58	118.90
1	Ba	524	U	C2-N1-C1'	6.13	125.05	117.70
1	Ba	1001	U	P-O3'-C3'	6.12	127.05	119.70
23	BA	1914	С	N3-C2-O2	-6.12	117.62	121.90
23	AA	882	С	C6-N1-C1'	-6.10	113.48	120.80
23	BA	2347	А	C2-N3-C4	6.10	113.65	110.60
23	BA	882	С	C6-N1-C1'	-6.10	113.48	120.80
1	Aa	502	С	C2-N1-C1'	6.10	125.51	118.80
1	Aa	460	А	C2-N3-C4	6.09	113.65	110.60
23	AA	575	G	C8-N9-C1'	-6.09	119.08	127.00
1	Aa	762	С	N1-C2-O2	6.09	122.56	118.90
1	Ba	762	С	N1-C2-O2	6.09	122.56	118.90
23	BA	575	G	C8-N9-C1'	-6.09	119.09	127.00
23	AA	593	U	C6-N1-C1'	-6.08	112.68	121.20
23	BA	2845	G	N3-C2-N2	-6.08	115.64	119.90
23	BA	593	U	C6-N1-C1'	-6.08	112.69	121.20
1	Ba	460	А	C2-N3-C4	6.07	113.64	110.60
1	Aa	162	А	C2-N3-C4	6.07	113.64	110.60
1	Aa	1140	С	N1-C2-O2	6.06	122.53	118.90
36	BN	15	LEU	CA-CB-CG	6.05	129.22	115.30
1	Ba	1140	С	N1-C2-O2	6.05	122.53	118.90
23	BA	2845	G	N3-C4-N9	-6.04	122.38	126.00
36	AN	15	LEU	CA-CB-CG	6.04	129.18	115.30
23	BA	2112	С	N1-C2-O2	6.03	122.52	118.90
24	AB	87	С	C6-N1-C2	-6.02	117.89	120.30
1	Aa	969	U	P-O3'-C3'	6.02	126.92	119.70
1	Aa	1314	G	P-O3'-C3'	6.02	126.92	119.70
23	AA	1179	С	C6-N1-C2	-6.02	117.89	120.30
23	AA	2347	A	C2-N3-C4	6.02	113.61	110.60
1	Ba	1314	G	P-O3'-C3'	6.02	126.92	119.70
23	BA	576	U	P-O3'-C3'	6.01	126.91	119.70
1	Ba	1096	U	C2-N1-C1'	6.01	124.91	117.70
23	BA	882	С	N1-C2-O2	6.00	122.50	118.90
1	Aa	1096	U	C2-N1-C1'	6.00	124.89	117.70
23	BA	882	С	N3-C2-O2	-6.00	117.70	121.90
23	BA	463	С	N1-C2-O2	6.00	122.50	118.90
23	AA	2112	С	N1-C2-O2	5.99	122.50	118.90
1	Ba	969	U	P-O3'-C3'	5.99	126.89	119.70
23	AA	576	U	P-O3'-C3'	5.96	126.86	119.70



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Ba	162	А	C2-N3-C4	5.96	113.58	110.60
23	BA	2223	С	C2-N1-C1'	5.96	125.35	118.80
1	Aa	1096	U	N1-C2-O2	5.95	126.97	122.80
23	AA	2223	С	C2-N1-C1'	5.95	125.34	118.80
23	BA	1179	С	C6-N1-C1'	-5.95	113.66	120.80
23	AA	1179	С	C6-N1-C1'	-5.94	113.67	120.80
23	AA	987	U	P-O3'-C3'	5.94	126.83	119.70
23	BA	987	U	P-O3'-C3'	5.94	126.83	119.70
31	AI	89	ASP	CB-CG-OD1	5.94	123.64	118.30
23	BA	1731	G	OP1-P-O3'	5.94	118.27	105.20
1	Ba	1096	U	N1-C2-O2	5.94	126.96	122.80
1	Ba	1267	А	P-O3'-C3'	5.94	126.82	119.70
23	AA	882	С	N3-C2-O2	-5.94	117.75	121.90
1	Aa	1267	А	P-O3'-C3'	5.93	126.82	119.70
23	AA	439	U	C6-N1-C1'	-5.93	112.89	121.20
23	AA	463	С	N1-C2-O2	5.93	122.46	118.90
23	BA	402	С	N1-C2-O2	5.93	122.46	118.90
23	AA	882	С	N1-C2-O2	5.93	122.46	118.90
1	Aa	1325	U	C2-N1-C1'	5.92	124.81	117.70
23	AA	1731	G	OP1-P-O3'	5.92	118.23	105.20
24	BB	100	U	C6-N1-C1'	-5.92	112.91	121.20
23	AA	577	А	P-O3'-C3'	5.91	126.80	119.70
1	Ba	1325	U	C2-N1-C1'	5.91	124.80	117.70
23	BA	439	U	C6-N1-C1'	-5.91	112.92	121.20
1	Aa	415	А	C2-N3-C4	5.91	113.55	110.60
23	BA	1179	С	C6-N1-C2	-5.90	117.94	120.30
23	AA	2049	U	N1-C2-O2	5.89	126.92	122.80
1	Aa	431	G	C8-N9-C1'	-5.89	119.34	127.00
24	AB	100	U	C6-N1-C1'	-5.89	112.95	121.20
1	Ba	431	G	C8-N9-C1'	-5.89	119.34	127.00
1	Ba	315	U	N1-C2-O2	5.89	126.92	122.80
23	BA	577	А	P-O3'-C3'	5.89	126.77	119.70
23	BA	2049	U	N1-C2-O2	5.89	126.92	122.80
1	Aa	315	U	N1-C2-O2	5.88	126.92	122.80
1	Aa	415	А	OP1-P-O3'	5.88	118.14	105.20
43	BU	53	ILE	C-N-CA	5.87	136.38	121.70
23	BA	897	Α	C5-C6-N6	-5.87	119.01	123.70
31	BI	89	ASP	CB-CG-OD1	5.86	123.58	118.30
1	Ba	599	U	N3-C2-O2	-5.86	118.10	122.20
1	Ba	387	С	N1-C2-O2	5.86	122.42	118.90
23	AA	402	С	N1-C2-O2	5.85	122.41	118.90
1	Ba	415	А	OP1-P-O3'	5.85	118.07	105.20



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
23	BA	2369	С	N1-C2-O2	5.85	122.41	118.90
23	BA	2370	U	N1-C2-O2	5.85	126.90	122.80
43	AU	53	ILE	C-N-CA	5.85	136.32	121.70
23	AA	897	А	C5-C6-N6	-5.84	119.03	123.70
23	BA	688	А	P-O3'-C3'	5.84	126.71	119.70
1	Aa	315	U	N3-C2-O2	-5.82	118.12	122.20
23	AA	2370	U	N1-C2-O2	5.82	126.88	122.80
1	Ba	315	U	N3-C2-O2	-5.82	118.12	122.20
1	Ba	415	А	C2-N3-C4	5.82	113.51	110.60
23	AA	1768	С	N1-C2-O2	5.82	122.39	118.90
23	BA	1768	С	N1-C2-O2	5.82	122.39	118.90
23	BA	2796	С	N1-C2-O2	5.82	122.39	118.90
24	BB	87	С	C6-N1-C2	-5.82	117.97	120.30
1	Aa	437	U	P-O3'-C3'	5.81	126.67	119.70
23	BA	828	А	C4-N9-C1'	5.81	136.76	126.30
1	Ba	437	U	P-O3'-C3'	5.80	126.67	119.70
23	AA	755	С	N1-C2-O2	5.80	122.38	118.90
23	AA	828	А	C4-N9-C1'	5.80	136.74	126.30
23	BA	268	А	O4'-C1'-N9	5.80	112.84	108.20
1	Aa	599	U	N3-C2-O2	-5.80	118.14	122.20
23	AA	688	А	P-O3'-C3'	5.80	126.66	119.70
23	AA	268	А	O4'-C1'-N9	5.79	112.83	108.20
1	Ba	1156	А	P-O3'-C3'	5.79	126.64	119.70
23	AA	2796	С	N1-C2-O2	5.78	122.37	118.90
23	AA	74	U	N3-C2-O2	-5.77	118.16	122.20
23	BA	74	U	N3-C2-O2	-5.77	118.16	122.20
23	AA	2742	С	N1-C2-O2	5.77	122.36	118.90
1	Aa	1156	А	P-O3'-C3'	5.77	126.62	119.70
23	BA	1287	U	N1-C2-O2	5.77	126.84	122.80
1	Aa	387	С	N1-C2-O2	5.76	122.36	118.90
1	Ba	336	С	N1-C2-O2	5.75	122.35	118.90
23	BA	2742	С	N1-C2-O2	5.75	122.35	118.90
1	Aa	336	С	N1-C2-O2	5.74	122.34	118.90
23	BA	755	С	N1-C2-O2	5.74	122.34	118.90
23	AA	1287	U	N1-C2-O2	5.73	126.81	122.80
$\overline{23}$	AA	1588	U	O4'-C1'-N1	5.73	112.78	108.20
23	AA	2369	С	N1-C2-O2	5.73	122.34	118.90
23	BA	1588	U	O4'-C1'-N1	5.72	112.78	108.20
23	AA	759	U	$C6-N1-\overline{C1'}$	-5.71	$113.2\overline{1}$	121.20
23	AA	943	C	N1-C2-O2	5.71	122.33	118.90
1	Ba	486	C	N1-C2-O2	5.71	122.32	118.90
23	BA	759	U	C6-N1-C1'	-5.69	113.23	121.20



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
23	AA	1213	С	N3-C2-O2	-5.69	117.92	121.90
23	AA	2361	U	N1-C2-O2	5.69	126.78	122.80
23	AA	1287	U	C2-N1-C1'	5.68	124.52	117.70
23	BA	862	С	C6-N1-C2	-5.68	118.03	120.30
1	Aa	486	С	N1-C2-O2	5.68	122.31	118.90
23	BA	943	С	N1-C2-O2	5.68	122.31	118.90
23	AA	2749	G	P-O3'-C3'	5.67	126.51	119.70
23	BA	1213	С	N3-C2-O2	-5.67	117.93	121.90
23	AA	975	U	N3-C2-O2	-5.67	118.23	122.20
23	BA	975	U	N3-C2-O2	-5.67	118.23	122.20
1	Ba	65	G	C4-N9-C1'	5.66	133.86	126.50
23	BA	2749	G	P-O3'-C3'	5.66	126.50	119.70
23	BA	1287	U	N3-C2-O2	-5.65	118.24	122.20
23	AA	1287	U	N3-C2-O2	-5.65	118.25	122.20
23	BA	1552	U	N1-C2-O2	5.64	126.75	122.80
23	AA	1803	G	C4-N9-C1'	5.64	133.83	126.50
23	BA	1803	G	C4-N9-C1'	5.64	133.83	126.50
1	Aa	1370	А	P-O3'-C3'	5.64	126.46	119.70
23	BA	1228	А	N7-C8-N9	5.63	116.62	113.80
23	BA	2370	U	C2-N1-C1'	5.63	124.46	117.70
23	AA	2370	U	C2-N1-C1'	5.63	124.45	117.70
1	Aa	599	U	C6-N1-C1'	-5.62	113.33	121.20
23	BA	1287	U	C2-N1-C1'	5.62	124.44	117.70
1	Aa	1136	U	P-O3'-C3'	5.62	126.44	119.70
23	AA	872	U	N1-C2-O2	5.62	126.73	122.80
1	Ba	1136	U	P-O3'-C3'	5.62	126.44	119.70
1	Ba	1370	А	P-O3'-C3'	5.62	126.44	119.70
1	Aa	65	G	C4-N9-C1'	5.62	133.80	126.50
23	AA	862	С	C6-N1-C2	-5.62	118.05	120.30
23	BA	1845	U	P-O3'-C3'	5.61	126.44	119.70
23	BA	593	U	C5-C6-N1	5.61	125.51	122.70
1	Ba	599	U	C6-N1-C1'	-5.60	113.36	121.20
23	BA	862	С	N3-C2-O2	-5.60	117.98	121.90
23	BA	1579	С	C6-N1-C2	-5.60	118.06	120.30
1	Ba	1048	С	N1-C2-O2	5.60	122.26	118.90
1	Ba	424	G	C8-N9-C1	-5.59	119.73	127.00
23	AA	1214	С	N3-C2-O2	-5.59	117.99	121.90
23	AA	1845	U	P-O3'-C3'	5.59	126.41	119.70
23	BA	1451	U	N1-C2-O2	5.59	126.71	122.80
23	AA	1552	U	N1-C2-O2	5.58	126.71	122.80
23	AA	593	U	C5-C6-N1	5.58	125.49	122.70
23	BA	872	U	N1-C2-O2	5.58	126.71	122.80



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
23	AA	1579	С	C6-N1-C2	-5.58	118.07	120.30
23	AA	1228	А	N7-C8-N9	5.58	116.59	113.80
23	AA	1633	А	C2-N3-C4	5.57	113.39	110.60
22	Av	153	MET	CG-SD-CE	-5.57	91.29	100.20
22	Bv	153	MET	CG-SD-CE	-5.57	91.29	100.20
1	Aa	424	G	C8-N9-C1'	-5.56	119.77	127.00
23	BA	2361	U	N1-C2-O2	5.56	126.69	122.80
23	AA	256	С	N1-C2-O2	5.56	122.24	118.90
23	AA	754	U	N1-C2-O2	5.56	126.69	122.80
23	BA	754	U	N1-C2-O2	5.56	126.69	122.80
23	AA	1343	U	C2-N1-C1'	5.56	124.37	117.70
23	AA	577	А	C2-N3-C4	5.56	113.38	110.60
23	BA	1214	С	N3-C2-O2	-5.56	118.01	121.90
23	AA	862	С	N3-C2-O2	-5.55	118.01	121.90
1	Aa	553	С	O4'-C1'-N1	5.55	112.64	108.20
23	AA	1692	С	C6-N1-C1'	-5.55	114.14	120.80
23	BA	1692	С	C6-N1-C1'	-5.55	114.14	120.80
1	Aa	1122	А	P-O3'-C3'	5.55	126.36	119.70
24	BB	69	С	N1-C2-O2	5.55	122.23	118.90
23	BA	2761	С	N1-C2-O2	5.54	122.23	118.90
1	Ba	1122	А	P-O3'-C3'	5.54	126.35	119.70
23	AA	1451	U	N1-C2-O2	5.54	126.68	122.80
23	BA	398	С	N1-C2-O2	5.54	122.22	118.90
35	BM	22	LEU	CA-CB-CG	5.54	128.04	115.30
35	AM	22	LEU	CA-CB-CG	5.54	128.03	115.30
1	Ba	387	С	N3-C2-O2	-5.54	118.03	121.90
23	BA	1343	U	C2-N1-C1'	5.54	124.34	117.70
23	AA	1992	С	N1-C2-O2	5.53	122.22	118.90
23	BA	1992	С	N1-C2-O2	5.53	122.22	118.90
23	BA	2699	U	N3-C2-O2	-5.52	118.33	122.20
23	BA	256	С	N1-C2-O2	5.52	122.21	118.90
23	AA	2761	С	N1-C2-O2	5.51	122.21	118.90
1	Ba	553	С	O4'-C1'-N1	5.51	112.61	108.20
23	AA	1894	G	C6-C5-N7	-5.50	127.10	130.40
1	Ba	55	С	C6-N1-C1'	-5.49	114.21	120.80
24	AB	69	С	N1-C2-O2	5.49	122.19	118.90
23	BA	1894	G	C6-C5-N7	-5.49	127.11	130.40
1	Aa	387	C	N3-C2-O2	-5.47	118.07	121.90
1	Ba	486	С	N3-C2-O2	-5.47	118.07	121.90
23	BA	2408	C	N1-C2-O2	5.47	122.18	118.90
23	AA	1049	С	N1-C2-O2	5.46	122.18	118.90
23	BA	2747	U	N3-C2-O2	-5.46	118.38	122.20



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
23	AA	1216	U	C2-N1-C1'	5.46	124.25	117.70
1	Aa	55	С	C6-N1-C1'	-5.46	114.25	120.80
23	AA	398	С	N1-C2-O2	5.46	122.17	118.90
23	BA	577	А	C2-N3-C4	5.45	113.33	110.60
23	BA	1049	С	N1-C2-O2	5.45	122.17	118.90
1	Aa	486	С	N3-C2-O2	-5.45	118.08	121.90
23	AA	2408	С	N1-C2-O2	5.45	122.17	118.90
23	AA	975	U	C2-N1-C1'	5.44	124.23	117.70
23	AA	872	U	N3-C2-O2	-5.43	118.40	122.20
23	AA	2699	U	N3-C2-O2	-5.43	118.39	122.20
23	BA	1633	А	C2-N3-C4	5.43	113.32	110.60
24	AB	115	С	N1-C2-O2	5.43	122.16	118.90
1	Ba	422	А	C2-N3-C4	5.43	113.31	110.60
1	Aa	1048	С	N1-C2-O2	5.42	122.16	118.90
23	BA	2321	С	N1-C2-O2	5.42	122.15	118.90
23	AA	1815	С	N1-C2-O2	5.42	122.15	118.90
1	Ba	1168	С	C2-N1-C1'	5.42	124.76	118.80
23	AA	327	G	O4'-C1'-N9	5.42	112.53	108.20
23	BA	327	G	O4'-C1'-N9	5.42	112.53	108.20
23	BA	1216	U	C2-N1-C1'	5.41	124.20	117.70
23	AA	575	G	N3-C4-C5	-5.41	125.90	128.60
23	BA	1815	С	N1-C2-O2	5.40	122.14	118.90
23	BA	975	U	C2-N1-C1'	5.40	124.17	117.70
24	BB	115	С	N1-C2-O2	5.39	122.14	118.90
1	Ba	411	С	C6-N1-C2	-5.38	118.15	120.30
23	AA	1101	А	C2-N3-C4	5.38	113.29	110.60
23	BA	1514	А	N1-C6-N6	5.38	121.83	118.60
1	Aa	1168	С	C2-N1-C1'	5.38	124.72	118.80
1	Ba	1157	С	N1-C2-O2	5.38	122.13	118.90
23	BA	1692	С	N3-C2-O2	-5.38	118.14	121.90
24	AB	100	U	N1-C2-O2	5.37	126.56	122.80
23	AA	1894	G	N3-C4-C5	-5.36	125.92	128.60
23	BA	1894	G	N3-C4-C5	-5.36	125.92	128.60
23	BA	1732	U	O5'-P-OP2	-5.36	100.88	105.70
23	AA	1514	А	N1-C6-N6	5.36	121.81	118.60
23	BA	460	C	N1-C2-O2	5.35	122.11	118.90
23	AA	2321	С	N1-C2-O2	5.35	122.11	118.90
23	AA	2361	U	N3-C2-O2	-5.35	118.46	122.20
1	Ba	55	С	C6-N1-C2	-5.35	118.16	120.30
23	AA	2747	U	N3-C2-O2	-5.34	118.46	122.20
23	BA	2731	С	N1-C2-O2	5.34	122.11	118.90
24	BB	94	С	N3-C2-O2	-5.34	118.16	121.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
23	BA	2249	G	O4'-C1'-N9	5.34	112.47	108.20
24	AB	94	С	N3-C2-O2	-5.33	118.17	121.90
25	AC	130	LEU	CA-CB-CG	5.33	127.56	115.30
25	BC	130	LEU	CA-CB-CG	5.33	127.56	115.30
23	AA	2049	U	N3-C2-O2	-5.33	118.47	122.20
1	Aa	1157	С	N1-C2-O2	5.33	122.10	118.90
23	AA	2731	С	N1-C2-O2	5.33	122.10	118.90
1	Aa	55	С	C6-N1-C2	-5.33	118.17	120.30
23	AA	971	U	N1-C2-O2	5.33	126.53	122.80
23	AA	1732	U	O5'-P-OP2	-5.33	100.91	105.70
23	BA	872	U	N3-C2-O2	-5.32	118.47	122.20
24	BB	100	U	N1-C2-O2	5.32	126.53	122.80
23	AA	2636	U	C2-N1-C1'	5.32	124.08	117.70
25	BC	19	LEU	CA-CB-CG	5.32	127.53	115.30
31	BI	64	ARG	CA-CB-CG	5.32	125.11	113.40
23	AA	988	С	N3-C2-O2	-5.32	118.18	121.90
23	AA	1692	С	N3-C2-O2	-5.32	118.18	121.90
1	Aa	411	С	C6-N1-C2	-5.31	118.17	120.30
31	AI	64	ARG	CA-CB-CG	5.31	125.09	113.40
25	AC	19	LEU	CA-CB-CG	5.31	127.52	115.30
23	BA	2112	С	N3-C2-O2	-5.31	118.18	121.90
23	AA	2112	С	N3-C2-O2	-5.30	118.19	121.90
23	AA	1551	U	O5'-P-OP1	-5.30	100.93	105.70
23	BA	1551	U	O5'-P-OP1	-5.30	100.93	105.70
23	BA	2636	U	C2-N1-C1'	5.30	124.06	117.70
23	AA	2249	G	O4'-C1'-N9	5.30	112.44	108.20
1	Aa	1012	G	C4-N9-C1'	5.29	133.37	126.50
23	BA	1101	А	C2-N3-C4	5.29	113.24	110.60
1	Ba	1012	G	C4-N9-C1'	5.29	133.37	126.50
23	BA	971	U	N1-C2-O2	5.29	126.50	122.80
23	AA	714	G	C4-N9-C1'	5.28	133.37	126.50
23	BA	714	G	C4-N9-C1'	5.28	133.37	126.50
23	BA	988	С	N3-C2-O2	-5.28	118.21	121.90
23	AA	394	U	N1-C2-O2	5.27	126.49	122.80
1	Aa	422	А	C2-N3-C4	5.27	113.23	110.60
23	BA	$39\overline{4}$	U	N1-C2-O2	$5.2\overline{7}$	126.49	122.80
23	AA	2263	C	N1-C2-O2	5.27	122.06	118.90
23	BA	575	G	N3-C4-C5	-5.26	125.97	128.60
23	BA	2361	U	N3-C2-O2	-5.26	118.52	122.20
23	BA	2049	U	N3-C2-O2	-5.26	118.52	122.20
23	BA	340	C	N1-C2-O2	5.25	122.05	118.90
23	AA	1758	А	C2-N3-C4	5.25	113.23	110.60



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
23	BA	1758	А	C2-N3-C4	5.25	113.23	110.60
23	AA	2796	С	N3-C2-O2	-5.25	118.22	121.90
23	BA	1451	U	N3-C2-O2	-5.25	118.52	122.20
23	BA	2263	С	N1-C2-O2	5.25	122.05	118.90
23	BA	2796	С	N3-C2-O2	-5.25	118.22	121.90
23	AA	460	С	N1-C2-O2	5.24	122.05	118.90
1	Ba	324	С	C6-N1-C2	-5.24	118.20	120.30
1	Ba	797	U	N1-C2-O2	5.24	126.47	122.80
1	Aa	502	С	N1-C2-O2	5.23	122.04	118.90
23	AA	340	С	N1-C2-O2	5.23	122.04	118.90
23	AA	1451	U	N3-C2-O2	-5.23	118.54	122.20
23	AA	1557	С	N1-C2-O2	5.22	122.03	118.90
23	BA	1557	С	N1-C2-O2	5.22	122.03	118.90
23	BA	1214	С	C2-N1-C1'	5.22	124.54	118.80
12	Al	62	LEU	CA-CB-CG	5.21	127.29	115.30
1	Ba	1186	А	C2-N3-C4	5.21	113.21	110.60
23	BA	1101	А	C4-N9-C1'	5.21	135.67	126.30
25	BC	13	ARG	CA-CB-CG	5.21	124.85	113.40
12	Bl	62	LEU	CA-CB-CG	5.20	127.27	115.30
1	Aa	1063	U	C2-N1-C1'	5.20	123.94	117.70
23	BA	1950	U	N1-C2-O2	5.20	126.44	122.80
1	Aa	1188	G	C4-N9-C1'	5.20	133.26	126.50
23	AA	1101	А	C4-N9-C1'	5.20	135.66	126.30
1	Ba	1063	U	C2-N1-C1'	5.20	123.94	117.70
23	AA	1101	А	N7-C8-N9	5.20	116.40	113.80
23	BA	1101	А	N7-C8-N9	5.20	116.40	113.80
1	Aa	1096	U	N3-C2-O2	-5.19	118.56	122.20
1	Ba	1096	U	N3-C2-O2	-5.19	118.56	122.20
25	AC	13	ARG	CA-CB-CG	5.19	124.82	113.40
23	AA	1950	U	N1-C2-O2	5.19	126.43	122.80
1	Aa	797	U	N1-C2-O2	5.18	126.43	122.80
23	BA	1953	U	N3-C2-O2	-5.18	118.57	122.20
32	BJ	61	LEU	CB-CG-CD2	-5.18	102.19	111.00
23	AA	1228	А	O4'-C1'-N9	5.18	112.34	108.20
32	AJ	6	LEU	CA-CB-CG	5.18	127.21	115.30
32	AJ	61	LEU	$CB-CG-\overline{CD2}$	-5.18	102.19	111.00
23	AA	754	U	N3-C2-O2	-5.18	118.58	122.20
23	BA	1228	А	O4'-C1'-N9	5.18	112.34	108.20
1	Ba	1188	G	C4-N9-C1'	5.18	133.23	126.50
32	BJ	6	LEU	CA-CB-CG	5.17	127.20	115.30
23	AA	1625	U	N3-C2-O2	-5.17	118.58	122.20
23	AA	1587	С	N1-C2-O2	5.16	122.00	118.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	Bf	54	ASP	CB-CG-OD1	5.16	122.94	118.30
1	Aa	1186	А	C2-N3-C4	5.16	113.18	110.60
23	AA	1385	G	P-O3'-C3'	5.15	125.88	119.70
23	AA	1953	U	N3-C2-O2	-5.15	118.59	122.20
23	AA	1214	С	C2-N1-C1'	5.15	124.46	118.80
23	AA	2263	С	C6-N1-C2	-5.15	118.24	120.30
23	BA	57	С	N1-C2-O2	5.15	121.99	118.90
1	Ba	542	U	C2-N1-C1'	5.14	123.87	117.70
23	AA	1160	С	N3-C2-O2	-5.14	118.30	121.90
1	Aa	1114	С	C6-N1-C2	-5.14	118.25	120.30
23	AA	57	С	N1-C2-O2	5.13	121.98	118.90
1	Aa	542	U	C2-N1-C1'	5.13	123.86	117.70
23	AA	256	С	N3-C2-O2	-5.13	118.31	121.90
23	AA	1651	С	N3-C2-O2	-5.13	118.31	121.90
23	BA	1160	С	N3-C2-O2	-5.13	118.31	121.90
23	AA	1761	G	N3-C4-C5	5.12	131.16	128.60
23	BA	1761	G	N3-C4-C5	5.12	131.16	128.60
23	BA	1651	С	N3-C2-O2	-5.12	118.31	121.90
1	Ba	797	U	N3-C2-O2	-5.12	118.62	122.20
23	BA	1385	G	P-O3'-C3'	5.12	125.84	119.70
23	BA	556	U	N1-C2-O2	5.12	126.38	122.80
23	BA	256	С	N3-C2-O2	-5.12	118.32	121.90
6	Af	54	ASP	CB-CG-OD1	5.11	122.90	118.30
24	AB	108	U	C6-N1-C1'	-5.11	114.04	121.20
1	Aa	99	U	C5-C6-N1	5.11	125.25	122.70
23	AA	1758	А	C4-N9-C1'	5.11	135.50	126.30
1	Aa	1373	А	C2-N3-C4	5.11	113.15	110.60
23	AA	576	U	C5-C6-N1	5.11	125.25	122.70
23	AA	1803	G	C8-N9-C1'	-5.11	120.36	127.00
1	Ba	1373	А	C2-N3-C4	5.11	113.15	110.60
23	BA	1803	G	C8-N9-C1'	-5.11	120.36	127.00
23	BA	2369	С	N3-C2-O2	-5.11	118.33	121.90
23	BA	1216	U	N1-C2-O2	5.10	126.37	122.80
23	BA	530	С	N1-C2-O2	5.10	121.96	118.90
23	BA	1587	С	N1-C2-O2	5.10	121.96	118.90
23	BA	2095	U	N1-C2-O2	5.10	126.37	122.80
23	AA	2819	C	C2-N1-C1'	5.09	124.41	118.80
23	BA	1758	A	C4-N9-C1'	5.09	135.47	126.30
24	BB	83	С	C6-N1-C2	-5.09	118.26	120.30
24	BB	108	U	C6-N1-C1'	-5.09	114.08	121.20
1	Aa	324	С	C6-N1-C2	-5.09	118.27	120.30
23	AA	1380	G	C4-N9-C1'	5.09	133.11	126.50



Mol	Chain	\mathbf{Res}	Type	Atoms		$Observed(^{o})$	$ $ Ideal(o)
23	BA	1828	U	N1-C2-O2	5.08	126.36	122.80
23	AA	2369	С	N3-C2-O2	-5.08	118.35	121.90
42	AT	82	LEU	C-N-CA	5.07	134.38	121.70
1	Aa	488	U	C2-N1-C1'	5.07	123.78	117.70
1	Ba	488	U	C2-N1-C1'	5.07	123.78	117.70
42	BT	82	LEU	C-N-CA	5.07	134.38	121.70
23	AA	556	U	N1-C2-O2	5.07	126.35	122.80
1	Ba	99	U	C5-C6-N1	5.07	125.23	122.70
1	Ba	502	С	N1-C2-O2	5.07	121.94	118.90
1	Aa	460	А	N3-C4-N9	5.06	131.44	127.40
23	AA	1552	U	C6-N1-C2	-5.06	117.97	121.00
23	BA	1552	U	C6-N1-C2	-5.06	117.97	121.00
23	AA	1828	U	N1-C2-O2	5.05	126.33	122.80
23	BA	576	U	C5-C6-N1	5.05	125.22	122.70
23	BA	593	U	N1-C2-O2	5.05	126.33	122.80
23	BA	402	С	N3-C2-O2	-5.05	118.37	121.90
23	BA	60	U	N1-C2-O2	5.04	126.33	122.80
1	Aa	99	U	P-O3'-C3'	5.04	125.75	119.70
23	BA	1380	G	C4-N9-C1'	5.04	133.06	126.50
23	BA	1625	U	N3-C2-O2	-5.04	118.67	122.20
23	AA	1992	С	N3-C2-O2	-5.04	118.37	121.90
1	Ba	460	А	N3-C4-N9	5.04	131.43	127.40
23	BA	1992	С	N3-C2-O2	-5.04	118.37	121.90
2	Ab	20	THR	C-N-CA	5.04	134.30	121.70
23	BA	2347	А	N3-C4-N9	5.04	131.43	127.40
23	BA	2223	С	C6-N1-C2	-5.04	118.28	120.30
23	BA	2819	С	C2-N1-C1'	5.04	124.34	118.80
23	AA	2095	U	N1-C2-O2	5.04	126.33	122.80
23	BA	754	U	N3-C2-O2	-5.04	118.67	122.20
23	AA	1132	А	O4'-C1'-N9	5.03	112.22	108.20
1	Ba	902	С	C6-N1-C1'	-5.03	114.76	120.80
24	AB	100	U	O4'-C1'-N1	5.03	112.22	108.20
1	Ba	99	U	P-O3'-C3'	5.03	125.73	119.70
23	BA	2263	С	C6-N1-C2	-5.03	118.29	120.30
1	Aa	797	U	N3-C2-O2	-5.03	118.68	122.20
23	AA	2224	U	N3-C2-O2	-5.03	118.68	122.20
23	AA	1559	G	N3-C2-N2	-5.02	116.38	119.90
23	BA	1559	G	N3-C2-N2	-5.02	116.38	119.90
23	AA	2223	C	C6-N1-C2	-5.02	118.29	120.30
23	AA	943	C	C6-N1-C2	-5.01	118.30	120.30
23	BA	1214	С	C6-N1-C2	-5.01	118.30	120.30
1	Aa	524	U	N3-C2-O2	-5.01	118.69	122.20



Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
23	AA	60	U	N1-C2-O2	5.01	126.31	122.80
23	AA	184	С	C5-C6-N1	5.01	123.50	121.00
1	Ba	1114	C	C6-N1-C2	-5.01	118.30	120.30
2	Bb	20	THR	C-N-CA	5.01	134.23	121.70
1	Aa	599	U	O4'-C1'-N1	5.01	112.20	108.20
23	AA	2347	A	N3-C4-N9	5.01	131.41	127.40
1	Ba	599	U	O4'-C1'-N1	5.01	112.20	108.20
35	AM	68	THR	C-N-CA	5.00	134.21	121.70
23	AA	460	C	C6-N1-C2	-5.00	118.30	120.30
1	Ba	65	G	OP2-P-O3'	5.00	116.20	105.20
23	BA	2224	U	N3-C2-O2	-5.00	118.70	122.20

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	AD	158	SER	Peptide
38	AP	50	ALA	Peptide
5	Ae	76	ARG	Peptide
9	Ai	108	ARG	Peptide
12	Al	126	GLY	Peptide
19	As	80	PHE	Peptide
20	At	58	ASP	Peptide
26	BD	158	SER	Peptide
38	BP	50	ALA	Peptide
5	Be	76	ARG	Peptide
9	Bi	108	ARG	Peptide
12	Bl	126	GLY	Peptide
19	Bs	80	PHE	Peptide
20	Bt	58	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.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
2	Ab	224/226~(99%)	209 (93%)	14 (6%)	1 (0%)	34	72
2	Bb	224/226~(99%)	208 (93%)	14 (6%)	2 (1%)	17	57
3	Ac	200/202~(99%)	177 (88%)	23 (12%)	0	100	100
3	Bc	200/202~(99%)	177 (88%)	23 (12%)	0	100	100
4	Ad	196/198~(99%)	170 (87%)	26 (13%)	0	100	100
4	Bd	196/198~(99%)	170 (87%)	26 (13%)	0	100	100
5	Ae	154/156~(99%)	147 (96%)	7 (4%)	0	100	100
5	Be	154/156~(99%)	147 (96%)	7 (4%)	0	100	100
6	Af	93/95~(98%)	85 (91%)	8 (9%)	0	100	100
6	Bf	93/95~(98%)	85 (91%)	8 (9%)	0	100	100
7	Ag	150/152~(99%)	144 (96%)	6 (4%)	0	100	100
7	Bg	150/152~(99%)	144 (96%)	6 (4%)	0	100	100
8	Ah	129/131~(98%)	122 (95%)	7 (5%)	0	100	100
8	Bh	129/131~(98%)	121 (94%)	8 (6%)	0	100	100
9	Ai	125/127~(98%)	112 (90%)	13 (10%)	0	100	100
9	Bi	125/127~(98%)	112 (90%)	13 (10%)	0	100	100
10	Aj	95/97~(98%)	88 (93%)	7 (7%)	0	100	100
10	Bj	95/97~(98%)	88 (93%)	7 (7%)	0	100	100
11	Ak	112/114~(98%)	93 (83%)	19 (17%)	0	100	100
11	Bk	112/114~(98%)	93 (83%)	19 (17%)	0	100	100
12	Al	133/135~(98%)	118 (89%)	15 (11%)	0	100	100
12	Bl	133/135~(98%)	118 (89%)	15 (11%)	0	100	100
13	Am	100/121~(83%)	90 (90%)	10 (10%)	0	100	100
13	Bm	100/121~(83%)	90 (90%)	10 (10%)	0	100	100
14	An	58/60~(97%)	49 (84%)	9 (16%)	0	100	100
14	Bn	58/60~(97%)	49 (84%)	9 (16%)	0	100	100
15	Ao	86/88~(98%)	85 (99%)	1 (1%)	0	100	100
15	Bo	86/88~(98%)	85 (99%)	1 (1%)	0	100	100
16	Ар	87/89~(98%)	78 (90%)	9 (10%)	0	100	100

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.



Chain Analysed Favoured Allowed Percentiles \mathbf{Mol} Outliers 100 100 1687/89 (98%) 78 (90%) 9(10%)0 Bp 100 100 0 1778/80 (98%) 72 (92%) 6(8%)Aq 100 1778/80 (98%) 72 (92%) 6(8%)0 100 Bq 18Ar 52/54 (96%) 51 (98%) 1(2%)0 100 100 100 1(2%)100 18 Br 52/54 (96%) 51 (98%) 0 19As78/80 (98%) 68 (87%) 10(13%)0 100 100 78/80 (98%) 100 100 19Bs69 (88%) 9(12%)0 77 (98%) 2(2%)0 100 100 20At 79/81 (98%) 20 Bt 79/81 (98%) 77 (98%) 2(2%)0 100 100 100 100 21Au 50/52 (96%) 48 (96%) 2(4%)0 100 100 21Bu 50/52 (96%) 48(96%)2(4%)0 22Av 158/190 (83%) 149(94%)9(6%)0 100 100 100 22Bv 158/190 (83%) 149(94%)9(6%)0 100 AC 100 100 25272/274 (99%) 257(94%)15(6%)0 25BC 272/274 (99%) 257 (94%) 15(6%)0 100 100 19(9%)100 100 26AD 213/215 (99%) 194 (91%)0 19(9%)0 100 26BD 213/215 (99%) 194 (91%)100 204/206 (99%) 192(94%)12(6%)100 100 27AE 0 100 100 27BE 204/206 (99%) 192(94%)12(6%)0 100 100 28AF 173/175 (99%) 142(82%)31 (18%) 0 142 (82%) 28BF 173/175 (99%) 31 (18%) 0 100 100 100 100 29AG 173/175 (99%) 155 (90%)18(10%)0 BG 100 29173/175 (99%) 155(90%)18(10%)0 100 30 AH 143/145 (99%) 131 (92%)12 (8%) 0 100 100 100 100 30 BH 143/145 (99%) 131 (92%)12(8%)0 31AI 120/122 (98%) 106 (88%) 14(12%)0 100 100 BI 106 (88%) 14(12%)0 100 100 31 120/122 (98%) AJ 144/146 (99%) 135(94%)9(6%)0 100 100 3232 BJ144/146 (99%) 135(94%)9 (6%) 0 100 100 100 100 AK 135/137 (98%) 127 (94%)8 (6%) 0 33 33 BK 127(94%)8 (6%) 0 100 100 135/137 (98%)



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
34	AL	118/120~(98%)	114 (97%)	4 (3%)	0	100	100
34	BL	118/120~(98%)	115 (98%)	3 (2%)	0	100	100
35	AM	117/119~(98%)	103 (88%)	14 (12%)	0	100	100
35	BM	117/119~(98%)	103 (88%)	14 (12%)	0	100	100
36	AN	112/114~(98%)	99 (88%)	13 (12%)	0	100	100
36	BN	112/114~(98%)	99 (88%)	13 (12%)	0	100	100
37	AO	114/116~(98%)	109 (96%)	5 (4%)	0	100	100
37	BO	114/116~(98%)	109 (96%)	5 (4%)	0	100	100
38	AP	100/102~(98%)	93 (93%)	6 (6%)	1 (1%)	15	54
38	BP	100/102~(98%)	93 (93%)	6 (6%)	1 (1%)	15	54
39	AQ	110/112~(98%)	106 (96%)	4 (4%)	0	100	100
39	BQ	110/112~(98%)	106 (96%)	4 (4%)	0	100	100
40	AR	87/89~(98%)	81 (93%)	6 (7%)	0	100	100
40	BR	87/89~(98%)	81 (93%)	6 (7%)	0	100	100
41	AS	101/103~(98%)	89 (88%)	12 (12%)	0	100	100
41	BS	101/103~(98%)	89 (88%)	12 (12%)	0	100	100
42	AT	92/94~(98%)	87 (95%)	5 (5%)	0	100	100
42	BT	92/94~(98%)	87 (95%)	5 (5%)	0	100	100
43	AU	80/82~(98%)	72 (90%)	8 (10%)	0	100	100
43	BU	80/82~(98%)	72 (90%)	8 (10%)	0	100	100
44	AV	56/58~(97%)	53~(95%)	3(5%)	0	100	100
44	BV	56/58~(97%)	53~(95%)	3(5%)	0	100	100
45	AW	65/67~(97%)	58 (89%)	7 (11%)	0	100	100
45	BW	65/67~(97%)	58 (89%)	7 (11%)	0	100	100
46	AX	56/58~(97%)	53~(95%)	3 (5%)	0	100	100
46	BX	56/58~(97%)	53~(95%)	3(5%)	0	100	100
47	AY	57/59~(97%)	45 (79%)	12 (21%)	0	100	100
47	BY	57/59~(97%)	45 (79%)	12 (21%)	0	100	100
48	AZ	$46/48 \ (96\%)$	40 (87%)	6 (13%)	0	100	100
48	BZ	46/48(96%)	40 (87%)	6 (13%)	0	100	100
49	A1	45/47~(96%)	44 (98%)	1 (2%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
49	B1	45/47~(96%)	44 (98%)	1 (2%)	0	100	100
50	A2	41/43~(95%)	39~(95%)	2(5%)	0	100	100
50	B2	41/43~(95%)	39~(95%)	2(5%)	0	100	100
51	A3	62/64~(97%)	58 (94%)	4 (6%)	0	100	100
51	B3	62/64~(97%)	57~(92%)	5 (8%)	0	100	100
52	A4	35/37~(95%)	35~(100%)	0	0	100	100
52	B4	35/37~(95%)	35~(100%)	0	0	100	100
All	All	11016/11310~(97%)	10097 (92%)	914 (8%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Ab	33	THR
38	AP	51	PRO
2	Bb	33	THR
38	BP	51	PRO
2	Bb	36	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	Ab	195/196~(100%)	194 (100%)	1 (0%)	88 93
2	Bb	195/196~(100%)	195 (100%)	0	100 100
3	Ac	138/164~(84%)	138 (100%)	0	100 100
3	Bc	138/164~(84%)	138 (100%)	0	100 100
4	Ad	147/174~(84%)	146~(99%)	1 (1%)	84 90
4	Bd	147/174~(84%)	146 (99%)	1 (1%)	84 90
5	Ae	118/122~(97%)	118 (100%)	0	100 100
5	Be	118/122~(97%)	118 (100%)	0	100 100



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
6	Af	80/83~(96%)	80 (100%)	0	100	100
6	Bf	80/83~(96%)	80 (100%)	0	100	100
7	Ag	118/128~(92%)	118 (100%)	0	100	100
7	Bg	118/128~(92%)	118 (100%)	0	100	100
8	Ah	111/112~(99%)	109 (98%)	2(2%)	59	77
8	Bh	111/112~(99%)	109 (98%)	2(2%)	59	77
9	Ai	86/105 (82%)	84 (98%)	2 (2%)	50	70
9	Bi	86/105 (82%)	84 (98%)	2 (2%)	50	70
10	Aj	81/87~(93%)	80 (99%)	1 (1%)	71	83
10	Bj	81/87~(93%)	80 (99%)	1 (1%)	71	83
11	Ak	82/90~(91%)	82 (100%)	0	100	100
11	Bk	82/90~(91%)	82 (100%)	0	100	100
12	Al	111/117~(95%)	110 (99%)	1 (1%)	78	87
12	Bl	111/117~(95%)	110 (99%)	1 (1%)	78	87
13	Am	62/104~(60%)	61 (98%)	1 (2%)	62	79
13	Bm	62/104~(60%)	61 (98%)	1 (2%)	62	79
14	An	48/52~(92%)	46 (96%)	2 (4%)	30	54
14	Bn	48/52~(92%)	46 (96%)	2 (4%)	30	54
15	Ao	77/80~(96%)	76~(99%)	1 (1%)	69	82
15	Bo	77/80~(96%)	76~(99%)	1 (1%)	69	82
16	Ap	73/75~(97%)	71 (97%)	2(3%)	44	65
16	Bp	73/75~(97%)	71 (97%)	2 (3%)	44	65
17	Aq	65/75~(87%)	65 (100%)	0	100	100
17	Bq	65/75~(87%)	65 (100%)	0	100	100
18	Ar	48/49~(98%)	48 (100%)	0	100	100
18	Br	48/49~(98%)	48 (100%)	0	100	100
19	As	67/70~(96%)	67 (100%)	0	100	100
19	Bs	67/70~(96%)	67 (100%)	0	100	100
20	At	61/67~(91%)	61 (100%)	0	100	100
20	Bt	61/67~(91%)	61 (100%)	0	100	100
21	Au	40/48~(83%)	40 (100%)	0	100	100



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
21	Bu	40/48~(83%)	40 (100%)	0	100	100
22	Av	147/173~(85%)	143~(97%)	4(3%)	44	65
22	Bv	147/173~(85%)	143~(97%)	4(3%)	44	65
25	AC	221/221~(100%)	221 (100%)	0	100	100
25	BC	221/221~(100%)	221 (100%)	0	100	100
26	AD	173/173~(100%)	172 (99%)	1 (1%)	86	92
26	BD	173/173~(100%)	172 (99%)	1 (1%)	86	92
27	AE	168/168~(100%)	167 (99%)	1 (1%)	86	92
27	BE	168/168~(100%)	167 (99%)	1 (1%)	86	92
28	AF	141/154 (92%)	139 (99%)	2 (1%)	67	80
28	BF	141/154 (92%)	139 (99%)	2 (1%)	67	80
29	AG	124/153~(81%)	122 (98%)	2 (2%)	62	79
29	BG	124/153~(81%)	122 (98%)	2 (2%)	62	79
30	AH	122/123~(99%)	121 (99%)	1 (1%)	81	89
30	BH	122/123~(99%)	121 (99%)	1 (1%)	81	89
31	AI	100/100~(100%)	99~(99%)	1 (1%)	76	86
31	BI	100/100~(100%)	99~(99%)	1 (1%)	76	86
32	AJ	109/112~(97%)	107~(98%)	2(2%)	59	77
32	BJ	109/112~(97%)	107 (98%)	2(2%)	59	77
33	AK	108/114~(95%)	107 (99%)	1 (1%)	78	87
33	BK	108/114~(95%)	107~(99%)	1 (1%)	78	87
34	AL	96/101~(95%)	95~(99%)	1 (1%)	76	86
34	BL	96/101~(95%)	95~(99%)	1 (1%)	76	86
35	AM	86/95~(90%)	83 (96%)	3 (4%)	36	59
35	BM	86/95~(90%)	83 (96%)	3 (4%)	36	59
36	AN	93/100~(93%)	92~(99%)	1 (1%)	73	84
36	BN	93/100~(93%)	92~(99%)	1 (1%)	73	84
37	AO	96/96~(100%)	95~(99%)	1 (1%)	76	86
37	BO	96/96~(100%)	95~(99%)	1 (1%)	76	86
38	AP	84/86~(98%)	84 (100%)	0	100	100
38	BP	84/86~(98%)	84 (100%)	0	100	100



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	AQ	89/91~(98%)	88~(99%)	1 (1%)	73	84
39	BQ	89/91~(98%)	88~(99%)	1 (1%)	73	84
40	AR	78/80~(98%)	76~(97%)	2(3%)	46	66
40	BR	78/80~(98%)	76~(97%)	2(3%)	46	66
41	AS	81/88~(92%)	80 (99%)	1 (1%)	71	83
41	BS	81/88~(92%)	80 (99%)	1 (1%)	71	83
42	AT	78/82~(95%)	78 (100%)	0	100	100
42	BT	78/82~(95%)	78 (100%)	0	100	100
43	AU	63/64~(98%)	60~(95%)	3(5%)	25	51
43	BU	63/64~(98%)	60~(95%)	3(5%)	25	51
44	AV	44/49~(90%)	43 (98%)	1 (2%)	50	70
44	BV	44/49~(90%)	43 (98%)	1 (2%)	50	70
45	AW	58/60~(97%)	58 (100%)	0	100	100
45	BW	58/60~(97%)	58 (100%)	0	100	100
46	AX	52/52~(100%)	52 (100%)	0	100	100
46	BX	52/52~(100%)	52~(100%)	0	100	100
47	AY	23/56~(41%)	23 (100%)	0	100	100
47	BY	23/56~(41%)	23~(100%)	0	100	100
48	AZ	35/44~(80%)	35 (100%)	0	100	100
48	ΒZ	35/44~(80%)	35 (100%)	0	100	100
49	A1	44/45~(98%)	44 (100%)	0	100	100
49	B1	44/45~(98%)	44 (100%)	0	100	100
50	A2	39/39~(100%)	39 (100%)	0	100	100
50	B2	39/39~(100%)	39 (100%)	0	100	100
51	A3	55/55~(100%)	55 (100%)	0	100	100
51	B3	55/55~(100%)	55 (100%)	0	100	100
52	A4	35/35~(100%)	34 (97%)	1 (3%)	42	64
52	B4	35/35~(100%)	34 (97%)	1 (3%)	42	64
All	All	8900/9614 (93%)	8813 (99%)	87 (1%)	77	86

All (87) residues with a non-rotameric sidechain are listed below:


Mol	Chain	\mathbf{Res}	Type
2	Ab	36	ASN
4	Ad	115	ASN
8	Ah	56	LYS
8	Ah	105	LEU
9	Ai	20	ARG
9	Ai	115	ARG
10	Aj	102	LEU
12	Al	44	ARG
13	Am	57	ARG
14	An	26	ARG
14	An	45	ARG
15	Ao	54	ARG
16	Ap	9	ARG
16	Ap	32	ARG
22	Av	103	ARG
22	Av	151	LEU
22	Av	164	THR
22	Av	179	ASP
26	AD	131	ILE
27	AE	193	VAL
28	AF	69	LYS
28	AF	125	ARG
29	AG	41	MET
29	AG	175	LYS
30	AH	97	ASN
31	AI	122	LEU
32	AJ	30	THR
32	AJ	114	ASN
33	AK	27	VAL
34	AL	29	ARG
35	AM	22	LEU
35	AM	35	ARG
35	AM	87	LYS
36	AN	11	THR
37	AO	4	VAL
39	AQ	98	LYS
40	AR	47	ASN
40	AR	56	MET
41	AS	8	ASN
43	AU	22	ARG
43	AU	61	ARG
43	AU	75	VAL
44	AV	60	THR



Mol	Chain	Res	Type
52	A4	35	ARG
4	Bd	115	ASN
8	Bh	56	LYS
8	Bh	105	LEU
9	Bi	20	ARG
9	Bi	115	ARG
10	Bj	102	LEU
12	Bl	44	ARG
13	Bm	57	ARG
14	Bn	26	ARG
14	Bn	45	ARG
15	Bo	54	ARG
16	Bp	9	ARG
16	Bp	32	ARG
22	Bv	103	ARG
22	Bv	151	LEU
22	Bv	164	THR
22	Bv	179	ASP
26	BD	131	ILE
27	BE	193	VAL
28	BF	69	LYS
28	BF	125	ARG
29	BG	41	MET
29	BG	175	LYS
30	BH	97	ASN
31	BI	122	LEU
32	BJ	30	THR
32	BJ	114	ASN
33	BK	27	VAL
34	BL	29	ARG
35	BM	22	LEU
$\overline{35}$	BM	35	ARG
35	BM	87	LYS
36	BN	11	THR
37	BO	4	VAL
39	BQ	98	LYS
40	BR	47	ASN
40	BR	56	MET
41	BS	8	ASN
43	BU	22	ARG
43	BU	61	ARG
43	BU	75	VAL



 $Continued \ from \ previous \ page...$

Mol	Chain	Res	Type
44	BV	60	THR
52	B4	35	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106) such sidechains are listed below:

Mol	Chain	Res	Type
2	Ab	190	ASN
3	Ac	53	HIS
3	Ac	64	ASN
4	Ad	115	ASN
4	Ad	146	GLN
5	Ae	83	HIS
6	Af	70	ASN
7	Ag	67	ASN
9	Ai	33	ASN
9	Ai	77	GLN
11	Ak	22	HIS
11	Ak	40	ASN
11	Ak	101	GLN
12	Al	42	GLN
12	Al	85	HIS
14	An	52	GLN
17	Aq	33	HIS
18	Ar	57	GLN
19	As	22	GLN
20	At	21	ASN
22	Av	82	ASN
22	Av	152	GLN
25	AC	86	ASN
25	AC	133	GLN
25	AC	230	HIS
26	AD	128	GLN
26	AD	148	HIS
26	AD	167	GLN
27	AE	75	GLN
28	AF	127	ASN
29	AG	77	GLN
30	AH	48	HIS
30	AH	97	ASN
31	AI	4	GLN
32	AJ	4	HIS
32	AJ	114	ASN



Mol	Chain	Res	Type
35	AM	43	GLN
36	AN	4	HIS
36	AN	79	HIS
37	AO	37	GLN
37	AO	91	ASN
38	AP	81	ASN
39	AQ	77	ASN
40	AR	47	ASN
41	AS	8	ASN
41	AS	39	ASN
41	AS	44	HIS
43	AU	20	ASN
44	AV	16	ASN
48	AZ	19	HIS
48	AZ	40	HIS
49	A1	26	ASN
49	A1	45	HIS
50	A2	17	HIS
2	Bb	190	ASN
3	Bc	53	HIS
3	Bc	64	ASN
4	Bd	115	ASN
4	Bd	146	GLN
5	Be	83	HIS
6	Bf	70	ASN
7	Bg	67	ASN
9	Bi	33	ASN
9	Bi	77	GLN
11	Bk	22	HIS
11	Bk	40	ASN
11	Bk	101	GLN
12	Bl	42	GLN
12	Bl	85	HIS
14	Bn	52	GLN
17	Bq	33	HIS
18	Br	57	GLN
19	Bs	22	GLN
20	Bt	21	ASN
22	Bv	152	GLN
25	BC	86	ASN
25	BC	133	GLN
25	BC	230	HIS



Mol	Chain	Res	Type
26	BD	128	GLN
26	BD	148	HIS
26	BD	167	GLN
27	BE	75	GLN
28	BF	127	ASN
29	BG	77	GLN
30	BH	48	HIS
30	BH	97	ASN
31	BI	4	GLN
32	BJ	4	HIS
32	BJ	114	ASN
35	BM	43	GLN
36	BN	4	HIS
36	BN	79	HIS
37	BO	37	GLN
37	BO	91	ASN
39	BQ	77	ASN
40	BR	47	ASN
41	BS	8	ASN
41	BS	39	ASN
41	BS	44	HIS
43	BU	20	ASN
44	BV	16	ASN
48	BZ	19	HIS
48	BZ	40	HIS
49	B1	26	ASN
49	B1	45	HIS
50	B2	17	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Aa	1537/1539~(99%)	470 (30%)	0
1	Ba	1537/1539~(99%)	468 (30%)	0
23	AA	2895/2923~(99%)	795~(27%)	27~(0%)
23	BA	2895/2923~(99%)	795~(27%)	28~(0%)
24	AB	113/115~(98%)	16 (14%)	0
24	BB	113/115~(98%)	16 (14%)	0
All	All	9090/9154 (99%)	2560~(28%)	55~(0%)

All (2560) RNA backbone outliers are listed below:



Mol	Chain	Res	Type
1	Aa	6	U
1	Aa	8	G
1	Aa	9	А
1	Aa	10	G
1	Aa	23	G
1	Aa	30	А
1	Aa	33	А
1	Aa	40	G
1	Aa	41	С
1	Aa	45	G
1	Aa	48	С
1	Aa	49	С
1	Aa	50	U
1	Aa	51	A
1	Aa	52	A
1	Aa	59	С
1	Aa	60	А
1	Aa	61	А
1	Aa	62	G
1	Aa	66	А
1	Aa	68	С
1	Aa	69	G
1	Aa	70	А
1	Aa	71	А
1	Aa	75	А
1	Aa	76	С
1	Aa	78	А
1	Aa	82	G
1	Aa	83	С
1	Aa	84	U
1	Aa	85	U
1	Aa	88	U
1	Aa	89	U
1	Aa	92	C
1	Aa	94	G
1	Aa	99	U
1	Aa	100	A
1	Aa	107	G
1	Aa	120	C
1	Aa	129	A
1	Aa	140	А
1	Aa	150	U
1	Aa	162	A



Mol	Chain	Res	Type
1	Aa	163	С
1	Aa	165	G
1	Aa	183	U
1	Aa	184	А
1	Aa	185	U
1	Aa	186	U
1	Aa	187	U
1	Aa	188	U
1	Aa	191	А
1	Aa	193	С
1	Aa	194	G
1	Aa	197	U
1	Aa	199	G
1	Aa	200	U
1	Aa	201	U
1	Aa	203	A
1	Aa	204	А
1	Aa	206	А
1	Aa	208	U
1	Aa	209	G
1	Aa	210	А
1	Aa	211	А
1	Aa	213	G
1	Aa	219	С
1	Aa	220	U
1	Aa	221	U
1	Aa	222	G
1	Aa	224	U
1	Aa	228	A
1	Aa	230	U
1	Aa	231	U
1	Aa	234	A
1	Aa	252	U
1	Aa	253	U
1	Aa	255	G
1	Aa	256	С
1	Aa	257	U
1	Aa	258	A
1	Aa	259	G
1	Aa	264	U
1	Aa	267	G
1	Aa	269	U



Mol	Chain	Res	Type
1	Aa	274	G
1	Aa	275	С
1	Aa	279	С
1	Aa	289	G
1	Aa	291	U
1	Aa	297	G
1	Aa	301	А
1	Aa	309	G
1	Aa	335	А
1	Aa	336	С
1	Aa	337	А
1	Aa	339	G
1	Aa	352	А
1	Aa	354	G
1	Aa	355	G
1	Aa	356	G
1	Aa	358	G
1	Aa	359	G
1	Aa	360	C
1	Aa	362	G
1	Aa	364	A
1	Aa	375	U
1	Aa	376	U
1	Aa	380	С
1	Aa	381	А
1	Aa	389	A
1	Aa	392	G
1	Aa	395	U
1	Aa	406	С
1	Aa	411	C
1	Aa	412	G
1	Aa	413	U
1	Aa	414	G
1	Aa	415	A
1	Aa	416	G
1	Aa	417	U
1	Aa	418	G
1	Aa	419	A
1	Aa	420	U
1	Aa	421	G
1	Aa	422	A
1	Aa	423	A



Mol	Chain	Res	Type
1	Aa	424	G
1	Aa	425	G
1	Aa	426	U
1	Aa	430	С
1	Aa	431	G
1	Aa	432	G
1	Aa	434	U
1	Aa	437	U
1	Aa	438	А
1	Aa	440	А
1	Aa	441	А
1	Aa	442	С
1	Aa	449	A
1	Aa	450	U
1	Aa	451	U
1	Aa	452	A
1	Aa	456	А
1	Aa	458	G
1	Aa	460	А
1	Aa	461	С
1	Aa	464	А
1	Aa	465	U
1	Aa	484	А
1	Aa	485	U
1	Aa	486	C
1	Aa	487	U
1	Aa	488	U
1	Aa	492	G
1	Aa	499	А
1	Aa	503	А
1	Aa	504	G
1	Aa	505	A
1	Aa	506	A
1	Aa	507	A
1	Aa	513	G
1	Aa	514	G
1	Aa	516	U
1	Aa	517	A
1	Aa	519	C
1	Aa	522	C
1	Aa	526	C
1	Aa	529	G



Mol	Chain	Res	Type
1	Aa	532	G
1	Aa	535	G
1	Aa	539	U
1	Aa	541	А
1	Aa	542	U
1	Aa	543	А
1	Aa	548	G
1	Aa	554	А
1	Aa	555	А
1	Aa	567	А
1	Aa	570	U
1	Aa	571	А
1	Aa	580	А
1	Aa	581	A
1	Aa	584	С
1	Aa	585	G
1	Aa	596	G
1	Aa	603	А
1	Aa	610	A
1	Aa	619	С
1	Aa	628	С
1	Aa	638	G
1	Aa	639	G
1	Aa	640	G
1	Aa	641	U
1	Aa	642	C
1	Aa	647	G
1	Aa	649	А
1	Aa	650	А
1	Aa	657	A
1	Aa	661	U
1	Aa	666	G
1	Aa	670	A
1	Aa	$67\overline{3}$	A
1	Aa	674	G
1	Aa	695	A
1	Aa	696	G
1	Aa	702	A
1	Aa	703	A
1	Aa	711	G
1	Aa	$71\overline{2}$	A
1	Aa	724	А



Mol	Chain	Res	Type
1	Aa	729	А
1	Aa	731	U
1	Aa	739	G
1	Aa	756	А
1	Aa	763	G
1	Aa	772	С
1	Aa	781	G
1	Aa	798	А
1	Aa	801	U
1	Aa	813	С
1	Aa	818	С
1	Aa	823	А
1	Aa	825	С
1	Aa	826	G
1	Aa	827	А
1	Aa	829	G
1	Aa	835	U
1	Aa	836	А
1	Aa	840	G
1	Aa	843	А
1	Aa	844	G
1	Aa	845	G
1	Aa	846	G
1	Aa	847	G
1	Aa	848	G
1	Aa	849	U
1	Aa	850	U
1	Aa	852	С
1	Aa	853	С
1	Aa	854	G
1	Aa	855	С
1	Aa	858	С
1	Aa	860	U
1	Aa	881	A
1	Aa	894	G
1	Aa	898	A
1	Aa	910	A
1	Aa	911	G
1	Aa	923	A
1	Aa	924	А
1	Aa	935	G
1	Aa	943	С



Mol	Chain	Res	Type
1	Aa	944	А
1	Aa	949	С
1	Aa	950	G
1	Aa	953	G
1	Aa	954	G
1	Aa	955	А
1	Aa	956	G
1	Aa	958	A
1	Aa	959	U
1	Aa	961	U
1	Aa	969	U
1	Aa	970	U
1	Aa	972	G
1	Aa	973	A
1	Aa	974	A
1	Aa	975	G
1	Aa	977	A
1	Aa	978	A
1	Aa	980	G
1	Aa	983	А
1	Aa	984	A
1	Aa	985	G
1	Aa	986	А
1	Aa	991	U
1	Aa	1001	U
1	Aa	1002	G
1	Aa	1003	A
1	Aa	1007	С
1	Aa	1008	С
1	Aa	1011	U
1	Aa	1012	G
1	Aa	1013	A
1	Aa	1015	A
1	Aa	1016	A
1	Aa	1017	С
1	Aa	1022	G
1	Aa	1023	А
1	Aa	1026	U
1	Aa	1032	С
1	Aa	1033	U
1	Aa	1035	С
1	Aa	1036	С



Mol	Chain	Res	Type
1	Aa	1038	С
1	Aa	1039	U
1	Aa	1041	С
1	Aa	1042	G
1	Aa	1043	G
1	Aa	1047	А
1	Aa	1048	С
1	Aa	1052	G
1	Aa	1055	А
1	Aa	1056	С
1	Aa	1057	А
1	Aa	1064	G
1	Aa	1065	С
1	Aa	1066	A
1	Aa	1076	U
1	Aa	1077	С
1	Aa	1091	А
1	Aa	1092	G
1	Aa	1094	U
1	Aa	1096	U
1	Aa	1101	U
1	Aa	1105	G
1	Aa	1106	U
1	Aa	1109	С
1	Aa	1112	А
1	Aa	1113	А
1	Aa	1115	G
1	Aa	1119	G
1	Aa	1123	С
1	Aa	1130	G
1	Aa	1135	G
1	Aa	1136	U
1	Aa	1137	U
1	Aa	1138	G
1	Aa	1141	А
1	Aa	1142	U
1	Aa	1143	C
1	Aa	1146	U
1	Aa	1148	А
1	Aa	1149	G
1	Aa	1150	U
1	Aa	1151	U



Mol	Chain	Res	Type
1	Aa	1154	G
1	Aa	1156	А
1	Aa	1157	С
1	Aa	1165	U
1	Aa	1167	А
1	Aa	1168	С
1	Aa	1169	U
1	Aa	1172	С
1	Aa	1173	G
1	Aa	1174	G
1	Aa	1175	U
1	Aa	1177	А
1	Aa	1178	С
1	Aa	1179	А
1	Aa	1181	А
1	Aa	1187	G
1	Aa	1188	G
1	Aa	1189	А
1	Aa	1190	А
1	Aa	1191	G
1	Aa	1194	G
1	Aa	1202	С
1	Aa	1203	G
1	Aa	1206	А
1	Aa	1207	А
1	Aa	1208	А
1	Aa	1209	U
1	Aa	1210	С
1	Aa	1211	А
1	Aa	1216	G
1	Aa	1222	U
1	Aa	1224	U
1	Aa	1225	G
1	Aa	1226	A
1	Aa	1228	U
1	Aa	1230	G
1	Aa	1234	U
1	Aa	1235	А
1	Aa	1236	C
1	Aa	1238	С
1	Aa	1243	G
1	Aa	1246	А



Mol	Chain	Res	Type
1	Aa	1248	А
1	Aa	1250	U
1	Aa	1251	G
1	Aa	1256	А
1	Aa	1260	А
1	Aa	1266	С
1	Aa	1267	А
1	Aa	1268	G
1	Aa	1270	G
1	Aa	1274	С
1	Aa	1275	С
1	Aa	1280	G
1	Aa	1281	G
1	Aa	1282	U
1	Aa	1283	С
1	Aa	1286	G
1	Aa	1287	С
1	Aa	1288	А
1	Aa	1289	А
1	Aa	1290	А
1	Aa	1291	U
1	Aa	1292	С
1	Aa	1296	U
1	Aa	1297	А
1	Aa	1300	G
1	Aa	1305	U
1	Aa	1307	U
1	Aa	1308	С
1	Aa	1309	А
1	Aa	1310	G
1	Aa	1311	U
1	Aa	1312	U
1	Aa	1313	С
1	Aa	1314	G
1	Aa	1315	G
1	Aa	1319	G
1	Aa	1320	U
1	Aa	1322	G
1	Aa	1327	С
1	Aa	1329	A
1	Aa	1332	С
1	Aa	1333	G



Mol	Chain	Res	Type
1	Aa	1335	С
1	Aa	1336	U
1	Aa	1337	А
1	Aa	1338	С
1	Aa	1339	А
1	Aa	1341	G
1	Aa	1345	С
1	Aa	1347	G
1	Aa	1348	G
1	Aa	1356	А
1	Aa	1357	G
1	Aa	1361	U
1	Aa	1363	G
1	Aa	1368	U
1	Aa	1371	G
1	Aa	1373	A
1	Aa	1378	А
1	Aa	1380	G
1	Aa	1387	А
1	Aa	1391	U
1	Aa	1392	С
1	Aa	1393	С
1	Aa	1404	A
1	Aa	1408	А
1	Aa	1419	С
1	Aa	1421	C
1	Aa	1428	А
1	Aa	1429	G
1	Aa	1438	А
1	Aa	1448	G
1	Aa	1451	G
1	Aa	1456	A
1	Aa	1461	U
1	Aa	1462	U
1	Aa	1463	U
1	Aa	1464	A
1	Aa	1466	G
1	Aa	1468	G
1	Aa	1476	U
1	Aa	1483	U
1	Aa	1495	U
1	Aa	1505	G



Mol	Chain	Res	Type
1	Aa	1508	G
1	Aa	1510	А
1	Aa	1514	А
1	Aa	1515	G
1	Aa	1540	G
1	Aa	1541	G
1	Aa	1543	U
23	AA	11	U
23	AA	15	G
23	AA	27	G
23	AA	28	А
23	AA	34	U
23	AA	36	G
23	AA	43	A
23	AA	51	G
23	AA	52	A
23	AA	53	А
23	AA	55	G
23	AA	63	U
23	AA	70	G
23	AA	71	А
23	AA	74	U
23	AA	75	G
23	AA	83	G
23	AA	84	А
23	AA	90	А
23	AA	92	G
23	AA	93	U
23	AA	96	G
23	AA	101	G
23	AA	102	A
23	AA	104	C
23	AA	117	A
23	AA	119	U
23	AA	124	A
23	AA	141	U
23	AA	148	U
23	AA	149	U
23	AA	152	С
23	AA	156	A
23	AA	157	U
23	AA	158	G



Mol	Chain	Res	Type
23	AA	161	А
23	AA	164	А
23	AA	167	U
23	AA	168	А
23	AA	170	С
23	AA	172	U
23	AA	173	А
23	AA	177	G
23	AA	178	А
23	AA	180	G
23	AA	184	C
23	AA	185	А
23	AA	199	A
23	AA	202	A
23	AA	213	С
23	AA	215	G
23	AA	216	А
23	AA	218	G
23	AA	219	А
23	AA	224	А
23	AA	225	А
23	AA	233	U
23	AA	246	U
23	AA	251	G
23	AA	255	G
23	AA	268	A
23	AA	269	G
23	AA	270	С
23	AA	279	А
23	AA	280	С
$\overline{23}$	AA	285	U
23	AA	286	U
23	AA	287	G
$\overline{23}$	AA	292	U
23	AA	293	U
23	AA	298	U
23	AA	299	U
23	AA	300	G
$\overline{23}$	AA	301	U
23	AA	302	A
23	AA	307	A
23	AA	309	U



Mol	Chain	Res	Type
23	AA	310	С
23	AA	311	U
23	AA	312	А
23	AA	316	G
23	AA	320	U
23	AA	321	U
23	AA	327	G
23	AA	328	G
23	AA	333	С
23	AA	335	U
23	AA	345	С
23	AA	353	А
23	AA	365	А
23	AA	366	G
23	AA	373	A
23	AA	388	A
23	AA	389	A
23	AA	392	U
23	AA	394	U
23	AA	397	U
23	AA	402	С
23	AA	404	U
23	AA	406	А
23	AA	410	G
23	AA	411	А
23	AA	417	А
23	AA	432	G
23	AA	435	А
23	AA	444	С
23	AA	447	A
23	AA	449	U
23	AA	451	U
23	AA	452	G
23	AA	458	A
23	AA	460	С
23	AA	481	C
23	AA	482	U
23	AA	486	G
23	AA	490	С
23	AA	492	G
23	AA	493	A
23	AA	501	С



Mol	Chain	Res	Type
23	AA	502	С
23	AA	503	А
23	AA	504	G
23	AA	506	А
23	AA	512	А
23	AA	513	G
23	AA	518	А
23	AA	523	А
23	AA	527	G
23	AA	535	G
23	AA	538	G
23	AA	539	G
23	AA	550	А
23	AA	553	A
23	AA	554	С
23	AA	557	G
23	AA	558	А
23	AA	559	А
23	AA	563	G
23	AA	566	U
23	AA	572	С
23	AA	574	А
23	AA	576	U
23	AA	577	А
23	AA	578	G
23	AA	580	С
23	AA	591	А
23	AA	592	А
23	AA	594	G
23	AA	606	G
23	AA	611	U
23	AA	616	G
23	AA	617	A
23	AA	618	А
23	AA	639	U
23	AA	644	C
23	AA	645	A
23	AA	646	A
23	AA	647	G
23	AA	659	A
$\overline{23}$	AA	672	A
23	AA	679	G



Mol	Chain	Res	Type
23	AA	682	А
23	AA	689	А
23	AA	690	U
23	AA	698	U
23	AA	699	U
23	AA	702	U
23	AA	713	А
23	AA	715	А
23	AA	720	А
23	AA	722	А
23	AA	730	А
23	AA	731	U
23	AA	735	С
23	AA	750	A
23	AA	754	U
23	AA	755	C
23	AA	759	U
23	AA	760	А
23	AA	761	А
23	AA	762	С
23	AA	763	А
23	AA	765	U
23	AA	766	G
23	AA	768	А
23	AA	771	G
23	AA	775	А
23	AA	792	U
23	AA	793	G
23	AA	797	А
23	AA	802	G
23	AA	809	А
23	AA	810	А
23	AA	816	G
23	AA	820	G
23	AA	822	G
23	AA	827	A
23	AA	829	U
23	AA	830	U
23	AA	834	A
23	AA	835	U
23	AA	836	С
23	AA	837	G



Mol	Chain	Res	Type
23	AA	840	С
23	AA	841	С
23	AA	842	U
23	AA	850	G
23	AA	856	U
23	AA	857	С
23	AA	868	А
23	AA	870	С
23	AA	872	U
23	AA	891	А
23	AA	892	U
23	AA	904	G
23	AA	911	А
23	AA	914	G
23	AA	918	G
23	AA	920	А
23	AA	926	G
23	AA	928	С
23	AA	940	U
23	AA	943	С
23	AA	949	С
23	AA	952	А
23	AA	955	А
23	AA	957	С
23	AA	960	С
23	AA	964	U
23	AA	968	А
23	AA	969	А
23	AA	970	U
23	AA	971	U
23	AA	972	А
23	AA	973	А
23	AA	975	U
23	AA	977	A
23	AA	985	А
23	AA	986	G
23	AA	988	С
23	AA	989	А
23	AA	990	G
23	AA	992	А
23	AA	997	G
23	AA	1003	А



Mol	Chain	Res	Type
23	AA	1005	G
23	AA	1012	G
23	AA	1018	А
23	AA	1019	А
23	AA	1024	А
23	AA	1025	А
23	AA	1027	А
23	AA	1034	А
23	AA	1040	А
23	AA	1043	U
23	AA	1047	G
23	AA	1049	С
23	AA	1056	U
23	AA	1057	А
23	AA	1066	G
23	AA	1067	U
23	AA	1069	G
23	AA	1070	А
23	AA	1076	А
23	AA	1077	U
23	AA	1078	G
23	AA	1086	G
23	AA	1087	С
23	AA	1088	С
23	AA	1089	С
23	AA	1091	G
23	AA	1092	А
23	AA	1093	С
23	AA	1094	А
23	AA	1095	А
23	AA	1100	G
23	AA	1102	U
23	AA	1105	U
23	AA	1106	G
23	AA	1109	U
23	AA	1111	А
23	AA	1113	А
23	AA	1114	А
23	AA	1115	G
23	AA	1116	С
23	AA	1117	А
23	AA	1118	G



Mol	Chain	Res	Type
23	AA	1119	С
23	AA	1120	С
23	AA	1122	U
23	AA	1126	U
23	AA	1127	U
23	AA	1128	А
23	AA	1132	А
23	AA	1133	G
23	AA	1137	G
23	AA	1138	U
23	AA	1139	А
23	AA	1140	А
23	AA	1143	G
23	AA	1145	U
23	AA	1148	С
23	AA	1150	А
23	AA	1151	G
23	AA	1155	А
23	AA	1156	G
23	AA	1158	G
23	AA	1160	С
23	AA	1161	А
23	AA	1162	С
23	AA	1163	U
23	AA	1174	U
23	AA	1176	U
23	AA	1178	С
23	AA	1179	С
23	AA	1186	А
23	AA	1200	А
23	AA	1201	G
23	AA	1208	А
23	AA	1214	C
$\overline{23}$	AA	1215	U
23	AA	1216	U
23	AA	1217	U
23	AA	1218	G
23	AA	1225	G
23	AA	1245	G
23	AA	1250	G
23	AA	1258	A
23	AA	1265	G



Mol	Chain	Res	Type
23	AA	1267	А
23	AA	1274	G
23	AA	1275	А
23	AA	1276	G
23	AA	1284	А
23	AA	1285	А
23	AA	1286	G
23	AA	1290	G
23	AA	1291	А
23	AA	1294	G
23	AA	1298	G
23	AA	1300	G
23	AA	1304	G
23	AA	1309	G
23	AA	1310	А
23	AA	1320	G
23	AA	1326	С
23	AA	1337	А
23	AA	1338	U
23	AA	1339	U
23	AA	1340	G
23	AA	1342	С
23	AA	1344	А
23	AA	1348	U
23	AA	1349	U
23	AA	1351	С
23	AA	1354	G
23	AA	1358	А
23	AA	1367	С
23	AA	1370	\mathbf{C}
23	AA	1386	U
23	AA	1387	С
23	AA	1389	U
23	AA	1392	G
23	AA	1394	U
23	AA	1402	A
23	AA	1405	G
23	AA	1415	A
23	AA	1416	U
23	AA	1417	G
23	AA	1420	U
23	AA	1422	A



Mol	Chain	Res	Type
23	AA	1423	С
23	AA	1432	А
23	AA	1440	А
23	AA	1443	А
23	AA	1445	С
23	AA	1447	А
23	AA	1450	А
23	AA	1451	U
23	AA	1453	G
23	AA	1454	U
23	AA	1455	U
23	AA	1457	U
23	AA	1459	A
23	AA	1463	А
23	AA	1464	U
23	AA	1471	А
23	AA	1472	С
23	AA	1481	А
23	AA	1489	А
23	AA	1490	G
23	AA	1491	С
23	AA	1494	G
23	AA	1495	С
23	AA	1496	G
23	AA	1497	А
23	AA	1498	U
23	AA	1499	U
23	AA	1503	U
23	AA	1504	U
23	AA	1510	U
23	AA	1516	С
23	AA	1518	G
23	AA	1519	U
23	AA	1520	A
23	AA	1521	А
$\overline{23}$	AA	1525	U
23	AA	1526	G
23	AA	$15\overline{27}$	A
23	AA	1532	U
23	AA	1533	A
$\overline{23}$	AA	1534	G
23	AA	1536	С



Mol	Chain	Res	Type
23	AA	1537	А
23	AA	1540	U
23	AA	1550	G
23	AA	1551	U
23	AA	1552	U
23	AA	1553	А
23	AA	1554	А
23	AA	1555	G
23	AA	1556	G
23	AA	1559	G
23	AA	1561	G
23	AA	1569	G
23	AA	1570	G
23	AA	1575	А
23	AA	1576	А
23	AA	1578	А
23	AA	1579	С
23	AA	1580	А
23	AA	1581	U
23	AA	1582	U
23	AA	1583	G
23	AA	1584	U
23	AA	1586	U
23	AA	1587	С
23	AA	1591	G
23	AA	1594	U
23	AA	1605	А
23	AA	1606	С
23	AA	1613	G
23	AA	1616	А
23	AA	1625	U
23	AA	1627	G
23	AA	1629	U
23	AA	1630	А
23	AA	1631	G
23	AA	1632	A
23	AA	1633	А
23	AA	1634	A
23	AA	1635	A
23	AA	1636	U
23	AA	1639	G
23	AA	1652	А



Mol	Chain	Res	Type
23	AA	1653	А
23	AA	1654	А
23	AA	1661	С
23	AA	1666	А
23	AA	1675	G
23	AA	1679	А
23	AA	1683	U
23	AA	1684	А
23	AA	1690	А
23	AA	1691	G
23	AA	1692	С
23	AA	1693	G
23	AA	1718	G
23	AA	1719	С
23	AA	1732	U
23	AA	1737	U
23	AA	1738	С
23	AA	1740	G
23	AA	1745	А
23	AA	1747	G
23	AA	1757	U
23	AA	1758	А
23	AA	1759	G
23	AA	1760	G
23	AA	1761	G
23	AA	1762	U
23	AA	1765	А
23	AA	1768	С
23	AA	1771	А
23	AA	1772	G
23	AA	1790	G
23	AA	1791	G
23	AA	1797	G
23	AA	1800	A
23	AA	1806	U
23	AA	1808	U
23	AA	1809	С
23	AA	1811	A
23	AA	1813	A
23	AA	1814	A
23	AA	1818	A
23	AA	1826	G



Mol	Chain	Res	Type
23	AA	1827	С
23	AA	1828	U
23	AA	1829	А
23	AA	1830	А
23	AA	1835	U
23	AA	1843	U
23	AA	1846	А
23	AA	1856	А
23	AA	1860	С
23	AA	1878	U
23	AA	1879	U
23	AA	1880	А
23	AA	1885	G
23	AA	1889	G
23	AA	1895	С
23	AA	1897	U
23	AA	1898	С
23	AA	1899	U
23	AA	1900	G
23	AA	1901	С
23	AA	1902	G
23	AA	1903	А
23	AA	1904	А
23	AA	1907	U
23	AA	1909	С
23	AA	1911	А
23	AA	1912	А
23	AA	1914	С
23	AA	1918	G
23	AA	1933	G
23	AA	1935	С
23	AA	1937	G
23	AA	1938	U
23	AA	1945	A
23	AA	1950	U
23	AA	1956	G
23	AA	1958	U
23	AA	1963	A
23	AA	1964	A
23	AA	1965	A
23	AA	1966	U
23	AA	1971	U



Mol	Chain	Res	Type
23	AA	1982	U
23	AA	1989	С
23	AA	1990	С
23	AA	1992	С
23	AA	1994	С
23	AA	1996	А
23	AA	1997	А
23	AA	1998	А
23	AA	1999	G
23	AA	2009	U
23	AA	2018	U
23	AA	2019	G
23	AA	2020	U
23	AA	2023	С
23	AA	2024	А
23	AA	2029	G
23	AA	2030	А
23	AA	2047	А
23	AA	2057	А
23	AA	2058	А
23	AA	2059	G
23	AA	2060	А
23	AA	2062	G
23	AA	2070	С
23	AA	2073	G
23	AA	2075	G
23	AA	2076	А
23	AA	2082	С
23	AA	2083	G
23	AA	2085	А
23	AA	2087	А
23	AA	2088	G
23	AA	2089	A
23	AA	2096	G
23	AA	$2\overline{097}$	G
23	AA	2103	U
23	AA	2107	G
23	AA	2109	A
23	AA	2110	G
23	AA	2111	С
23	AA	2115	A
23	AA	$2\overline{117}$	A



Mol	Chain	Res	Type
23	AA	2118	U
23	AA	2119	U
23	AA	2120	G
23	AA	2126	С
23	AA	2129	С
23	AA	2139	А
23	AA	2140	С
23	AA	2143	G
23	AA	2145	U
23	AA	2147	G
23	AA	2153	А
23	AA	2155	С
23	AA	2157	U
23	AA	2158	U
23	AA	2160	G
23	AA	2161	А
23	AA	2164	С
23	AA	2172	С
23	AA	2173	U
23	AA	2174	А
23	AA	2175	G
23	AA	2176	С
23	AA	2183	G
23	AA	2185	А
23	AA	2186	G
23	AA	2188	С
23	AA	2190	С
23	AA	2193	G
23	AA	2194	U
23	AA	2195	G
23	AA	2198	A
23	AA	2204	С
23	AA	2215	U
23	AA	2224	U
23	AA	$2\overline{2}25$	A
23	AA	2229	С
23	AA	2230	G
23	AA	$2\overline{231}$	С
23	AA	2232	A
23	AA	2238	U
23	AA	2240	U
23	AA	2241	С



Mol	Chain	Res	Type
23	AA	2243	U
23	AA	2252	А
23	AA	2261	G
23	AA	2262	G
23	AA	2263	С
23	AA	2265	G
23	AA	2266	G
23	AA	2290	С
23	AA	2295	А
23	AA	2305	А
23	AA	2306	G
23	AA	2310	С
23	AA	2314	А
23	AA	2316	G
23	AA	2321	С
23	AA	2328	А
23	AA	2329	U
23	AA	2330	G
23	AA	2331	G
23	AA	2332	U
23	AA	2333	U
23	AA	2334	G
23	AA	2335	G
23	AA	2336	А
23	AA	2337	А
23	AA	2345	A
23	AA	2346	U
23	AA	2347	А
23	AA	2352	G
23	AA	2353	U
23	AA	2358	G
23	AA	2361	U
23	AA	2362	A
23	AA	2370	U
23	AA	2374	С
23	AA	2377	C
23	AA	2385	А
23	AA	2388	A
23	AA	2396	A
23	AA	2409	G
23	AA	2410	G
23	AA	2411	А



Mol	Chain	Res	Type
23	AA	2412	С
23	AA	2429	U
23	AA	2433	С
23	AA	2434	А
23	AA	2441	G
23	AA	2449	С
23	AA	2450	U
23	AA	2451	С
23	AA	2455	G
23	AA	2456	G
23	AA	2457	А
23	AA	2458	U
23	AA	2459	А
23	AA	2460	А
23	AA	2461	А
23	AA	2462	А
23	AA	2463	G
23	AA	2468	С
23	AA	2472	G
23	AA	2474	G
23	AA	2475	А
23	AA	2485	U
23	AA	2486	А
23	AA	2503	А
23	AA	2511	G
23	AA	2521	G
23	AA	2525	С
23	AA	2529	G
23	AA	2530	А
23	AA	2531	U
23	AA	2532	G
23	AA	2540	A
23	AA	2544	С
23	AA	2545	А
23	AA	2547	С
23	AA	2556	G
23	AA	2561	С
23	AA	2562	G
23	AA	2568	A
23	AA	2569	А
23	AA	2570	G
23	AA	2581	U



Mol	Chain	Res	Type
23	AA	2589	U
23	AA	2592	А
23	AA	2593	А
23	AA	2594	G
23	AA	2599	А
23	AA	2600	С
23	AA	2604	А
23	AA	2605	G
23	AA	2613	С
23	AA	2626	G
23	AA	2629	А
23	AA	2630	G
23	AA	2636	U
23	AA	2640	U
23	AA	2642	U
23	AA	2646	U
23	AA	2648	G
23	AA	2650	G
23	AA	2656	А
23	AA	2657	G
23	AA	2666	А
23	AA	2672	G
23	AA	2679	U
23	AA	2681	А
23	AA	2687	А
23	AA	2692	А
23	AA	2695	G
23	AA	2696	G
23	AA	2697	G
23	AA	2699	U
23	AA	2700	G
23	AA	2712	G
23	AA	2716	U
23	AA	2741	G
23	AA	2745	G
23	AA	2750	С
23	AA	2753	U
23	AA	2756	G
23	AA	2757	U
23	AA	2759	G
23	AA	2760	А
23	AA	2761	С



Mol	Chain	Res	Type
23	AA	2764	G
23	AA	2769	G
23	AA	2771	G
23	AA	2775	А
23	AA	2778	G
23	AA	2784	А
23	AA	2788	А
23	AA	2793	G
23	AA	2794	С
23	AA	2796	С
23	AA	2798	С
23	AA	2800	U
23	AA	2801	С
23	AA	2803	А
23	AA	2804	G
23	AA	2805	A
23	AA	2806	U
23	AA	2808	А
23	AA	2817	А
23	AA	2820	U
23	AA	2821	U
23	AA	2822	С
23	AA	2823	G
23	AA	2824	G
23	AA	2827	А
23	AA	2828	U
23	AA	2829	А
23	AA	2831	G
23	AA	2832	А
23	AA	2838	С
23	AA	2840	А
23	AA	2843	А
23	AA	2850	G
23	AA	2853	U
23	AA	2854	А
23	AA	2855	A
23	AA	2879	G
23	AA	2887	G
23	AA	2888	A
23	AA	2892	G
23	AA	2899	A
23	AA	2900	С



23 AA 2903 A 23 AA 2913 G 23 AA 2914 A 23 AA 2919 A 24 AB 10 U 24 AB 22 G 24 AB 23 U 24 AB 23 U 24 AB 23 U 24 AB 33 U 24 AB 33 U 24 AB 33 U 24 AB 33 U 24 AB 39 G 24 AB 40 C 24 AB 55 A 24 AB 55 A 24 AB 87 C 24 AB 88 G 24 AB 110 C 24 AB 113 G 1 Ba 6 U 1 Ba	Mol	Chain	Res	Type
23AA2913G23AA2914A23AA2919A24AB10U24AB22G24AB23U24AB23U24AB24C24AB33U24AB33U24AB33U24AB33U24AB33G24AB55A24AB55A24AB55A24AB64A24AB87C24AB88G24AB113G24AB113G24AB113G24AB113G24AB113G1Ba8G1Ba9A1Ba30A1Ba33A1Ba33A1Ba40G1Ba44C1Ba45G1Ba49C1Ba50U1Ba50C1Ba50C1Ba50C1Ba60A	23	AA	2903	А
23AA2914A23AA2919A24AB10U24AB22G24AB23U24AB23U24AB24C24AB33U24AB39G24AB39G24AB40C24AB43A24AB51A24AB55A24AB87C24AB88G24AB116G24AB88G24AB113G24AB113G24AB113G24AB113G24AB113G24AB113G1Ba6U1Ba9A1Ba30A1Ba33A1Ba40G1Ba41C1Ba44C1Ba50U1Ba51A1Ba59C1Ba59C1Ba60A	23	AA	2913	G
23AA2919A24AB10U24AB22G24AB23U24AB24C24AB33U24AB39G24AB39G24AB40C24AB43A24AB55A24AB55A24AB64A24AB87C24AB88G24AB110C24AB13G24AB13G24AB13G24AB106G24AB113G1Ba6U1Ba9A1Ba30A1Ba33A1Ba40G1Ba40G1Ba44C1Ba44C1Ba45G1Ba50U1Ba51A1Ba52A1Ba59C1Ba60A	23	AA	2914	А
24AB10U 24 AB 22 G 24 AB 23 U 24 AB 24 C 24 AB 33 U 24 AB 33 U 24 AB 39 G 24 AB 40 C 24 AB 43 A 24 AB 51 A 24 AB 55 A 24 AB 64 A 24 AB 64 A 24 AB 87 C 24 AB 88 G 24 AB 106 G 24 AB 111 C 24 AB 113 G 1 Ba 6 U 1 Ba 6 U 1 Ba 6 U 1 Ba 30 A 1 Ba 33 A 1 Ba 33 A 1 Ba 33 A 1 Ba 40 G 1 Ba 44 C 1 Ba 44 C 1 Ba 49 C 1 Ba 50 U 1 Ba 50 U 1 Ba 50 C 1 Ba 50 <	23	AA	2919	А
24 AB 22 G 24 AB 23 U 24 AB 24 C 24 AB 33 U 24 AB 39 G 24 AB 39 G 24 AB 40 C 24 AB 43 A 24 AB 55 A 24 AB 55 A 24 AB 64 A 24 AB 87 C 24 AB 88 G 24 AB 106 G 24 AB 110 C 24 AB 111 C 24 AB 113 G 1 Ba 6 U 1 Ba 9 A 1 Ba 9 A 1 Ba 30 A 1 Ba 40 </td <td>24</td> <td>AB</td> <td>10</td> <td>U</td>	24	AB	10	U
24 AB 23 U 24 AB 33 U 24 AB 33 U 24 AB 39 G 24 AB 40 C 24 AB 43 A 24 AB 51 A 24 AB 55 A 24 AB 64 A 24 AB 64 A 24 AB 87 C 24 AB 87 C 24 AB 106 G 24 AB 106 G 24 AB 113 G 1 Ba 6 U 1 Ba 6 U 1 Ba 6 U 1 Ba 6 U 1 Ba 30 A 1 Ba 33 A 1 Ba 45	24	AB	22	G
24AB 24 C 24 AB 33 U 24 AB 39 G 24 AB 40 C 24 AB 43 A 24 AB 51 A 24 AB 55 A 24 AB 64 A 24 AB 87 C 24 AB 88 G 24 AB 88 G 24 AB 88 G 24 AB 106 G 24 AB 110 C 24 AB 111 C 24 AB 106 G 24 AB 106 G 24 AB 110 G 1 Ba 6 U 1 Ba 6 U 1 Ba 6 U 1 Ba 30 A 1 Ba 30 A 1 Ba 33 A 1 Ba 40 G 1 Ba 44 C 1 Ba 44 C 1 Ba 49 C 1 Ba 50 U 1 Ba 52 A 1 Ba 59 C 1 Ba 50 A	24	AB	23	U
24 AB 33 U 24 AB 40 C 24 AB 43 A 24 AB 51 A 24 AB 51 A 24 AB 55 A 24 AB 64 A 24 AB 64 A 24 AB 87 C 24 AB 87 C 24 AB 88 G 24 AB 106 G 24 AB 106 G 24 AB 111 C 24 AB 113 G 1 Ba 6 U 1 Ba 9 A 1 Ba 9 A 1 Ba 30 A 1 Ba 30 A 1 Ba 40 G 1 Ba 49 <td>24</td> <td>AB</td> <td>24</td> <td>С</td>	24	AB	24	С
24AB 39 G 24 AB 40 C 24 AB 43 A 24 AB 51 A 24 AB 55 A 24 AB 64 A 24 AB 87 C 24 AB 87 C 24 AB 88 G 24 AB 106 G 24 AB 111 C 24 AB 113 G 24 AB 113 G 24 AB 113 G 24 AB 113 G 1 Ba 6 U 1 Ba 6 U 1 Ba 30 A 1 Ba 30 A 1 Ba 30 A 1 Ba 33 A 1 Ba 41 C 1 Ba 45 G 1 Ba 49 C 1 Ba 50 U 1 Ba 50 U 1 Ba 50 C 1 Ba 59 C 1 Ba 59 C 1 Ba 60 A	24	AB	33	U
24 AB 40 C 24 AB 51 A 24 AB 55 A 24 AB 64 A 24 AB 64 A 24 AB 64 A 24 AB 87 C 24 AB 87 C 24 AB 88 G 24 AB 106 G 24 AB 111 C 24 AB 111 C 24 AB 111 C 24 AB 111 C 24 AB 113 G 1 Ba 6 U 1 Ba 9 A 1 Ba 30 A 1 Ba 33 A 1 Ba 44 C 1 Ba 49	24	AB	39	G
24AB43A 24 AB51A 24 AB55A 24 AB64A 24 AB87C 24 AB88G 24 AB106G 24 AB111C 24 AB113G 24 AB113G 1 Ba6U1Ba8G1Ba9A1Ba30A1Ba30A1Ba40G1Ba45G1Ba48C1Ba49C1Ba50U1Ba51A1Ba52A1Ba59C1Ba60A	24	AB	40	С
24AB 51 A 24 AB 55 A 24 AB 64 A 24 AB 87 C 24 AB 88 G 24 AB 106 G 24 AB 111 C 24 AB 113 G1Ba 6 U1Ba 6 U1Ba 9 A1Ba 10 G1Ba 10 G1Ba 30 A1Ba 33 A1Ba 41 C1Ba 45 G1Ba 49 C1Ba 50 U1Ba 51 A1Ba 59 C1Ba 59 C1Ba 60 A	24	AB	43	А
24AB 55 A 24 AB 64 A 24 AB 87 C 24 AB 88 G 24 AB 106 G 24 AB 111 C 24 AB 111 C 24 AB 111 C 24 AB 113 G 1 Ba 6 U 1 Ba 6 U 1 Ba 9 A 1 Ba 9 A 1 Ba 30 A 1 Ba 30 A 1 Ba 30 A 1 Ba 40 G 1 Ba 41 C 1 Ba 45 G 1 Ba 49 C 1 Ba 50 U 1 Ba 51 A 1 Ba 52 A 1 Ba 59 C 1 Ba 60 A	24	AB	51	А
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$2\overline{4}$	AB	55	A
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	24	AB	64	А
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	24	AB	87	С
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	24	AB	88	G
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	24	AB	106	G
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	24	AB	111	С
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	24	AB	113	G
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Ba	6	U
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Ba	8	G
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	Ba	9	А
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	Ba	10	G
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	Ba	23	G
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	Ba	30	А
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	Ba	33	A
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Ba	40	G
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Ba	41	С
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	Ba	45	G
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Ba	48	C
1 Ba 50 U 1 Ba 51 A 1 Ba 52 A 1 Ba 59 C 1 Ba 60 A	1	Ba	49	С
1 Ba 51 A 1 Ba 52 A 1 Ba 59 C 1 Ba 60 A	1	Ba	50	U
1 Ba 52 A 1 Ba 59 C 1 Ba 60 A	1	Ba	51	A
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Ba	52	A
1 Ba 60 A	1	Ba	$\overline{59}$	C
	1	Ba	60	А
1 Ba 61 A	1	Ba	61	A
1 Ba 62 G	1	Ba	62	G
1 Ba 66 A	1	Ba	66	A
1 Ba 68 C	1	Ba	68	C
1 Ba 69 G	1	Ba	69	G


1 Ba 70 A 1 Ba 71 A 1 Ba 75 A 1 Ba 76 C 1 Ba 78 A 1 Ba 82 G 1 Ba 83 C 1 Ba 84 U 1 Ba 84 U 1 Ba 85 U 1 Ba 89 U 1 Ba 92 C 1 Ba 94 G 1 Ba 100 A 1 Ba 100 A 1 Ba 100 A 1 Ba 100 A 1 Ba 120 C 1 Ba 120 C 1 Ba 162 A 1 Ba 165 G 1 Ba 165 G 1 Ba 188	Mol	Chain	Res	Type
1 Ba 71 A 1 Ba 75 A 1 Ba 76 C 1 Ba 78 A 1 Ba 82 G 1 Ba 83 C 1 Ba 83 C 1 Ba 84 U 1 Ba 85 U 1 Ba 89 U 1 Ba 92 C 1 Ba 94 G 1 Ba 99 U 1 Ba 100 A 1 Ba 120 C 1 Ba 129 A 1 Ba 162 A 1 Ba 163 C 1 Ba 165 G 1 Ba 185 U 1 Ba 185 U 1 Ba 186 U 1 Ba 191	1	Ba	70	А
1 Ba 75 A 1 Ba 76 C 1 Ba 78 A 1 Ba 82 G 1 Ba 83 C 1 Ba 83 C 1 Ba 84 U 1 Ba 84 U 1 Ba 85 U 1 Ba 89 U 1 Ba 92 C 1 Ba 99 U 1 Ba 99 U 1 Ba 100 A 1 Ba 100 A 1 Ba 100 A 1 Ba 100 A 1 Ba 120 C 1 Ba 162 A 1 Ba 165 G 1 Ba 165 G 1 Ba 185 U 1 Ba 186	1	Ba	71	А
1 Ba 76 C 1 Ba 78 A 1 Ba 82 G 1 Ba 83 C 1 Ba 83 C 1 Ba 84 U 1 Ba 85 U 1 Ba 89 U 1 Ba 92 C 1 Ba 92 C 1 Ba 94 G 1 Ba 99 U 1 Ba 100 A 1 Ba 100 A 1 Ba 100 A 1 Ba 100 A 1 Ba 120 C 1 Ba 120 C 1 Ba 162 A 1 Ba 165 G 1 Ba 165 G 1 Ba 185 U 1 Ba 186	1	Ba	75	А
1 Ba 78 A 1 Ba 82 G 1 Ba 83 C 1 Ba 84 U 1 Ba 85 U 1 Ba 89 U 1 Ba 89 U 1 Ba 92 C 1 Ba 94 G 1 Ba 99 U 1 Ba 99 U 1 Ba 100 A 1 Ba 100 A 1 Ba 120 C 1 Ba 120 C 1 Ba 120 A 1 Ba 162 A 1 Ba 163 C 1 Ba 163 C 1 Ba 185 U 1 Ba 185 U 1 Ba 186 U 1 Ba 191	1	Ba	76	С
1 Ba 82 G 1 Ba 83 C 1 Ba 84 U 1 Ba 85 U 1 Ba 88 U 1 Ba 89 U 1 Ba 92 C 1 Ba 94 G 1 Ba 94 G 1 Ba 99 U 1 Ba 100 A 1 Ba 120 C 1 Ba 120 C 1 Ba 162 A 1 Ba 163 C 1 Ba 165 G 1 Ba 185 U 1 Ba 186 U 1 Ba 191	1	Ba	78	А
1 Ba 83 C 1 Ba 84 U 1 Ba 85 U 1 Ba 88 U 1 Ba 89 U 1 Ba 92 C 1 Ba 92 C 1 Ba 92 C 1 Ba 94 G 1 Ba 99 U 1 Ba 100 A 1 Ba 100 A 1 Ba 120 C 1 Ba 120 C 1 Ba 120 A 1 Ba 120 A 1 Ba 162 A 1 Ba 163 C 1 Ba 165 G 1 Ba 185 U 1 Ba 185 U 1 Ba 191 A 1 Ba 191	1	Ba	82	G
1Ba 84 U1Ba 85 U1Ba 88 U1Ba 92 C1Ba 92 C1Ba 94 G1Ba 99 U1Ba 100 A1Ba 100 A1Ba 100 A1Ba 120 C1Ba 120 C1Ba 120 C1Ba 120 C1Ba 162 A1Ba 162 A1Ba 165 G1Ba 165 G1Ba 183 U1Ba 185 U1Ba 185 U1Ba 186 U1Ba 193 C1Ba 193 C1Ba 194 G1Ba 197 U1Ba 197 U1Ba 200 U1Ba 200 U1Ba 204 A1Ba 206 A1Ba 206 A1Ba 209 G1Ba 209 G1Ba 209 G1Ba 209 G1Ba 209 G1Ba 209 G </td <td>1</td> <td>Ba</td> <td>83</td> <td>С</td>	1	Ba	83	С
1 Ba 85 U 1 Ba 89 U 1 Ba 92 C 1 Ba 94 G 1 Ba 94 G 1 Ba 99 U 1 Ba 100 A 1 Ba 107 G 1 Ba 120 C 1 Ba 129 A 1 Ba 129 A 1 Ba 150 U 1 Ba 162 A 1 Ba 163 C 1 Ba 165 G 1 Ba 183 U 1 Ba 185 U 1 Ba 185 U 1 Ba 187 U 1 Ba 193 C 1 Ba 194 G 1 Ba 199 G 1 Ba 199 <td>1</td> <td>Ba</td> <td>84</td> <td>U</td>	1	Ba	84	U
1 Ba 88 U 1 Ba 92 C 1 Ba 94 G 1 Ba 99 U 1 Ba 100 A 1 Ba 100 A 1 Ba 107 G 1 Ba 120 C 1 Ba 129 A 1 Ba 129 A 1 Ba 120 C 1 Ba 120 C 1 Ba 129 A 1 Ba 162 A 1 Ba 163 C 1 Ba 163 C 1 Ba 183 U 1 Ba 185 U 1 Ba 186 U 1 Ba 191 A 1 Ba 193 C 1 Ba 194 G 1 Ba 199<	1	Ba	85	U
1Ba 89 U1Ba 92 C1Ba 94 G1Ba 99 U1Ba 100 A1Ba 100 A1Ba 107 G1Ba 120 C1Ba 120 C1Ba 120 C1Ba 120 C1Ba 120 C1Ba 120 C1Ba 140 A1Ba 162 A1Ba 165 G1Ba 165 G1Ba 183 U1Ba 185 U1Ba 185 U1Ba 186 U1Ba 191 A1Ba 193 C1Ba 194 G1Ba 197 U1Ba 197 U1Ba 200 U1Ba 200 U1Ba 203 A1Ba 204 A1Ba 206 A1Ba 208 U1Ba 209 G1Ba 209 G1Ba 200 A	1	Ba	88	U
1Ba92C1Ba94G1Ba99U1Ba100A1Ba107G1Ba120C1Ba129A1Ba140A1Ba150U1Ba162A1Ba163C1Ba165G1Ba183U1Ba185U1Ba185U1Ba186U1Ba187U1Ba191A1Ba193C1Ba194G1Ba197U1Ba199G1Ba200U1Ba203A1Ba204A1Ba208U1Ba208U1Ba209G1Ba209G	1	Ba	89	U
1Ba 94 G1Ba 99 U1Ba 100 A1Ba 107 G1Ba 120 C1Ba 120 C1Ba 129 A1Ba 140 A1Ba 150 U1Ba 162 A1Ba 163 C1Ba 165 G1Ba 183 U1Ba 184 A1Ba 184 A1Ba 184 U1Ba 186 U1Ba 187 U1Ba 191 A1Ba 193 C1Ba 197 U1Ba 197 U1Ba 200 U1Ba 200 U1Ba 203 A1Ba 204 A1Ba 204 A1Ba 208 U1Ba 208 U1Ba 209 G1Ba 209 G	1	Ba	92	С
1Ba99U1Ba100A1Ba107G1Ba120C1Ba129A1Ba140A1Ba150U1Ba162A1Ba163C1Ba163G1Ba183U1Ba185G1Ba185U1Ba186U1Ba187U1Ba193C1Ba194G1Ba197U1Ba199G1Ba200U1Ba203A1Ba204A1Ba208U1Ba208U1Ba208U1Ba209G1Ba209G	1	Ba	94	G
1Ba100A1Ba107G1Ba120C1Ba129A1Ba140A1Ba140A1Ba162A1Ba162A1Ba163C1Ba165G1Ba183U1Ba184A1Ba185U1Ba186U1Ba187U1Ba191A1Ba193C1Ba194G1Ba197U1Ba200U1Ba201U1Ba203A1Ba204A1Ba206A1Ba208U1Ba209G1Ba209G	1	Ba	99	U
1Ba 107 G1Ba 120 C1Ba 129 A1Ba 140 A1Ba 150 U1Ba 162 A1Ba 163 C1Ba 163 C1Ba 183 U1Ba 185 U1Ba 185 U1Ba 185 U1Ba 186 U1Ba 187 U1Ba 187 U1Ba 191 A1Ba 193 C1Ba 194 G1Ba 197 U1Ba 197 U1Ba 200 U1Ba 203 A1Ba 204 A1Ba 208 U1Ba 208 U1Ba 208 U1Ba 209 G1Ba 209 G1Ba 209 G1Ba 209 G1Ba 209 G	1	Ba	100	A
1Ba120C1Ba129A1Ba140A1Ba150U1Ba162A1Ba163C1Ba165G1Ba183U1Ba184A1Ba185U1Ba185U1Ba186U1Ba187U1Ba191A1Ba193C1Ba194G1Ba197U1Ba199G1Ba200U1Ba203A1Ba204A1Ba206A1Ba208U1Ba209G1Ba209G1Ba209G	1	Ba	107	G
1Ba129A1Ba140A1Ba150U1Ba162A1Ba163C1Ba163G1Ba183U1Ba185G1Ba185U1Ba186U1Ba187U1Ba193C1Ba193C1Ba194G1Ba197U1Ba200U1Ba201U1Ba203A1Ba204A1Ba206A1Ba208U1Ba209G1Ba209G1Ba209G1Ba209G	1	Ba	120	С
1Ba140A1Ba150U1Ba162A1Ba163C1Ba165G1Ba183U1Ba184A1Ba185U1Ba186U1Ba187U1Ba188U1Ba193C1Ba194G1Ba197U1Ba199G1Ba200U1Ba203A1Ba203A1Ba204A1Ba206A1Ba208U1Ba209G1Ba209G1Ba209G1Ba210A	1	Ba	129	A
1Ba150U1Ba162A1Ba163C1Ba165G1Ba183U1Ba184A1Ba185U1Ba186U1Ba187U1Ba193C1Ba193C1Ba194G1Ba197U1Ba199G1Ba200U1Ba203A1Ba204A1Ba206A1Ba208U1Ba209G1Ba209G1Ba209G1Ba209G1Ba210A	1	Ba	140	А
1Ba162A1Ba163C1Ba165G1Ba183U1Ba184A1Ba185U1Ba186U1Ba187U1Ba187U1Ba191A1Ba193C1Ba194G1Ba197U1Ba199G1Ba200U1Ba203A1Ba204A1Ba206A1Ba208U1Ba209G1Ba209G1Ba210A	1	Ba	150	U
1Ba163C1Ba165G1Ba183U1Ba184A1Ba185U1Ba186U1Ba187U1Ba187U1Ba191A1Ba193C1Ba194G1Ba197U1Ba199G1Ba200U1Ba201U1Ba203A1Ba204A1Ba206A1Ba208U1Ba209G1Ba209G1Ba210A	1	Ba	162	A
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Ba	163	С
1 Ba 183 U 1 Ba 184 A 1 Ba 185 U 1 Ba 185 U 1 Ba 186 U 1 Ba 187 U 1 Ba 187 U 1 Ba 187 U 1 Ba 197 U 1 Ba 193 C 1 Ba 193 C 1 Ba 193 C 1 Ba 193 C 1 Ba 194 G 1 Ba 197 U 1 Ba 200 U 1 Ba 201 U 1 Ba 203 A 1 Ba 204 A 1 Ba 206 A 1 Ba 208 U 1 Ba 209 G 1 Ba	1	Ba	165	G
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Ba	183	U
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Ba	184	A
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Ba	185	U
1 Ba 187 U 1 Ba 188 U 1 Ba 191 A 1 Ba 193 C 1 Ba 193 C 1 Ba 193 C 1 Ba 194 G 1 Ba 197 U 1 Ba 199 G 1 Ba 200 U 1 Ba 201 U 1 Ba 203 A 1 Ba 204 A 1 Ba 206 A 1 Ba 208 U 1 Ba 209 G 1 Ba 209 G 1 Ba 210 A	1	Ba	186	U
1 Ba 188 U 1 Ba 191 A 1 Ba 193 C 1 Ba 194 G 1 Ba 197 U 1 Ba 197 U 1 Ba 199 G 1 Ba 200 U 1 Ba 201 U 1 Ba 203 A 1 Ba 204 A 1 Ba 206 A 1 Ba 208 U 1 Ba 209 G 1 Ba 209 A	1	Ba	187	U
1 Ba 191 A 1 Ba 193 C 1 Ba 194 G 1 Ba 197 U 1 Ba 199 G 1 Ba 200 U 1 Ba 200 U 1 Ba 201 U 1 Ba 203 A 1 Ba 204 A 1 Ba 206 A 1 Ba 208 U 1 Ba 209 G 1 Ba 209 A	1	Ba	188	U
1 Ba 193 C 1 Ba 194 G 1 Ba 197 U 1 Ba 199 G 1 Ba 199 G 1 Ba 200 U 1 Ba 201 U 1 Ba 203 A 1 Ba 204 A 1 Ba 206 A 1 Ba 208 U 1 Ba 209 G 1 Ba 210 A	1	Ba	191	A
1 Ba 194 G 1 Ba 197 U 1 Ba 199 G 1 Ba 200 U 1 Ba 201 U 1 Ba 203 A 1 Ba 204 A 1 Ba 206 A 1 Ba 208 U 1 Ba 209 G 1 Ba 210 A	1	Ba	193	С
1 Ba 197 U 1 Ba 199 G 1 Ba 200 U 1 Ba 201 U 1 Ba 203 A 1 Ba 204 A 1 Ba 206 A 1 Ba 208 U 1 Ba 209 G 1 Ba 210 A	1	Ba	194	G
1 Ba 199 G 1 Ba 200 U 1 Ba 201 U 1 Ba 203 A 1 Ba 204 A 1 Ba 206 A 1 Ba 208 U 1 Ba 209 G 1 Ba 210 A	1	Ba	197	U
1 Ba 200 U 1 Ba 201 U 1 Ba 203 A 1 Ba 204 A 1 Ba 206 A 1 Ba 208 U 1 Ba 209 G 1 Ba 210 A	1	Ba	199	G
1 Ba 201 U 1 Ba 203 A 1 Ba 204 A 1 Ba 206 A 1 Ba 208 U 1 Ba 209 G 1 Ba 210 A	1	Ba	200	U
1 Ba 203 A 1 Ba 204 A 1 Ba 206 A 1 Ba 208 U 1 Ba 209 G 1 Ba 210 A	1	Ba	201	U
1 Ba 204 A 1 Ba 206 A 1 Ba 208 U 1 Ba 209 G 1 Ba 210 A	1	Ba	203	A
1 Ba 206 A 1 Ba 208 U 1 Ba 209 G 1 Ba 210 A	1	Ba	204	A
1 Ba 208 U 1 Ba 209 G 1 Ba 210 A	1	Ba	206	A
1 Ba 209 G 1 Ba 210 A	1	Ba	208	U
1 Ba 210 A	1	Ba	209	G
	1	Ba	210	А



1 Ba 211 A 1 Ba 213 G 1 Ba 219 C 1 Ba 220 U 1 Ba 221 U 1 Ba 222 G 1 Ba 222 G
1 Ba 213 G 1 Ba 219 C 1 Ba 220 U 1 Ba 221 U 1 Ba 222 G 1 Ba 222 G
1 Ba 219 C 1 Ba 220 U 1 Ba 221 U 1 Ba 222 G 1 Ba 222 G
1 Ba 220 U 1 Ba 221 U 1 Ba 222 G 1 Ba 222 G
1 Ba 221 U 1 Ba 222 G 1 Ba 224 U
1 Ba 222 G
1 D_{π} 004 U
1 Ba 224 U
1 Ba 228 A
1 Ba 230 U
1 Ba 231 U
1 Ba 234 A
1 Ba 252 U
1 Ba 253 U
1 Ba 255 G
1 Ba 256 C
1 Ba 257 U
1 Ba 258 A
1 Ba 259 G
1 Ba 264 U
1 Ba 267 G
1 Ba 269 U
1 Ba 274 G
1 Ba 275 C
1 Ba 279 C
1 Ba 289 G
1 Ba 291 U
1 Ba 297 G
1 Ba 301 A
1 Ba 309 G
1 Ba 335 A
1 Ba 336 C
1 Ba 337 A
1 Ba 339 G
1 Ba 352 A
1 Ba 354 G
1 Ba 355 G
1 Ba 356 G
1 Ba 358 G
1 Ba 359 G
1 Ba 360 C
1 Ba 362 G
1 Ba 364 A



Mol	Chain	Res	Type
1	Ba	375	U
1	Ba	376	U
1	Ba	380	С
1	Ba	381	А
1	Ba	389	А
1	Ba	392	G
1	Ba	395	U
1	Ba	406	С
1	Ba	411	С
1	Ba	412	G
1	Ba	413	U
1	Ba	414	G
1	Ba	415	А
1	Ba	416	G
1	Ba	417	U
1	Ba	418	G
1	Ba	419	А
1	Ba	420	U
1	Ba	421	G
1	Ba	422	A
1	Ba	423	A
1	Ba	424	G
1	Ba	425	G
1	Ba	426	U
1	Ba	430	С
1	Ba	431	G
1	Ba	432	G
1	Ba	434	U
1	Ba	437	U
1	Ba	438	A
1	Ba	440	А
1	Ba	441	A
1	Ba	442	С
1	Ba	449	A
1	Ba	450	U
1	Ba	451	U
1	Ba	452	A
1	Ba	456	A
1	Ba	458	G
1	Ba	460	A
1	Ba	461	C
1	Ba	464	А



Mol	Chain	Res	Type
1	Ba	465	U
1	Ba	484	А
1	Ba	485	U
1	Ba	486	С
1	Ba	487	U
1	Ba	488	U
1	Ba	492	G
1	Ba	499	A
1	Ba	503	A
1	Ba	504	G
1	Ba	505	А
1	Ba	506	A
1	Ba	507	A
1	Ba	513	G
1	Ba	514	G
1	Ba	516	U
1	Ba	517	A
1	Ba	519	С
1	Ba	522	С
1	Ba	526	С
1	Ba	529	G
1	Ba	532	G
1	Ba	535	G
1	Ba	539	U
1	Ba	541	A
1	Ba	542	U
1	Ba	543	A
1	Ba	548	G
1	Ba	554	A
1	Ba	555	А
1	Ba	567	A
1	Ba	570	U
1	Ba	571	A
1	Ba	580	A
1	Ba	581	А
1	Ba	584	С
1	Ba	585	G
1	Ba	596	G
1	Ba	603	А
1	Ba	610	A
1	Ba	619	C
1	Ba	628	С



Mol	Chain	Res	Type
1	Ba	638	G
1	Ba	639	G
1	Ba	640	G
1	Ba	641	U
1	Ba	642	С
1	Ba	647	G
1	Ba	649	А
1	Ba	650	А
1	Ba	657	А
1	Ba	661	U
1	Ba	666	G
1	Ba	670	A
1	Ba	673	А
1	Ba	674	G
1	Ba	695	А
1	Ba	696	G
1	Ba	702	А
1	Ba	703	А
1	Ba	711	G
1	Ba	712	А
1	Ba	724	А
1	Ba	729	A
1	Ba	731	U
1	Ba	739	G
1	Ba	756	A
1	Ba	763	G
1	Ba	772	C
1	Ba	781	G
1	Ba	798	A
1	Ba	801	U
1	Ba	813	С
1	Ba	818	С
1	Ba	823	A
1	Ba	825	С
1	Ba	826	G
1	Ba	827	А
1	Ba	829	G
1	Ba	835	U
1	Ba	836	А
1	Ba	840	G
1	Ba	845	G
1	Ba	847	G



Mol	Chain	Res	Type
1	Ba	848	G
1	Ba	849	U
1	Ba	850	U
1	Ba	852	С
1	Ba	853	С
1	Ba	854	G
1	Ba	855	С
1	Ba	856	С
1	Ba	857	С
1	Ba	858	С
1	Ba	881	А
1	Ba	894	G
1	Ba	898	А
1	Ba	910	A
1	Ba	911	G
1	Ba	923	A
1	Ba	924	A
1	Ba	935	G
1	Ba	943	С
1	Ba	944	А
1	Ba	949	С
1	Ba	950	G
1	Ba	953	G
1	Ba	954	G
1	Ba	955	A
1	Ba	956	G
1	Ba	958	A
1	Ba	959	U
1	Ba	961	U
1	Ba	969	U
1	Ba	970	U
1	Ba	972	G
1	Ba	973	A
1	Ba	974	A
1	Ba	975	G
1	Ba	977	А
1	Ba	978	A
1	Ba	980	G
1	Ba	983	А
1	Ba	984	A
1	Ba	985	G
1	Ba	986	А



Mol	Chain	Res	Type
1	Ba	991	U
1	Ba	1001	U
1	Ba	1002	G
1	Ba	1003	А
1	Ba	1007	С
1	Ba	1008	С
1	Ba	1011	U
1	Ba	1012	G
1	Ba	1013	А
1	Ba	1015	А
1	Ba	1016	А
1	Ba	1017	С
1	Ba	1022	G
1	Ba	1023	A
1	Ba	1026	U
1	Ba	1032	С
1	Ba	1033	U
1	Ba	1035	С
1	Ba	1036	С
1	Ba	1038	С
1	Ba	1039	U
1	Ba	1041	С
1	Ba	1042	G
1	Ba	1043	G
1	Ba	1047	А
1	Ba	1048	С
1	Ba	1052	G
1	Ba	1055	А
1	Ba	1056	С
1	Ba	1057	А
1	Ba	1064	G
1	Ba	1065	C
1	Ba	1066	А
1	Ba	1076	U
1	Ba	1077	С
1	Ba	1091	А
1	Ba	1092	G
1	Ba	1094	U
1	Ba	1096	U
1	Ba	1101	U
1	Ba	1105	G
1	Ba	1106	U



Mol	Chain	Res	Type
1	Ba	1109	С
1	Ba	1112	А
1	Ba	1113	А
1	Ba	1115	G
1	Ba	1119	G
1	Ba	1123	С
1	Ba	1130	G
1	Ba	1135	G
1	Ba	1136	U
1	Ba	1137	U
1	Ba	1138	G
1	Ba	1141	А
1	Ba	1142	U
1	Ba	1143	С
1	Ba	1146	U
1	Ba	1148	A
1	Ba	1149	G
1	Ba	1150	U
1	Ba	1151	U
1	Ba	1154	G
1	Ba	1156	А
1	Ba	1157	С
1	Ba	1165	U
1	Ba	1167	А
1	Ba	1168	С
1	Ba	1169	U
1	Ba	1172	С
1	Ba	1173	G
1	Ba	1174	G
1	Ba	1175	U
1	Ba	1177	А
1	Ba	1178	C
1	Ba	1179	А
1	Ba	1181	A
1	Ba	1187	G
1	Ba	1188	G
1	Ba	1189	А
1	Ba	1190	А
1	Ba	1191	G
1	Ba	1194	G
1	Ba	1202	C
1	Ba	1203	G



Mol	Chain	Res	Type
1	Ba	1206	А
1	Ba	1207	А
1	Ba	1208	А
1	Ba	1209	U
1	Ba	1210	С
1	Ba	1211	А
1	Ba	1216	G
1	Ba	1222	U
1	Ba	1224	U
1	Ba	1225	G
1	Ba	1226	А
1	Ba	1228	U
1	Ba	1230	G
1	Ba	1234	U
1	Ba	1235	А
1	Ba	1236	С
1	Ba	1238	С
1	Ba	1243	G
1	Ba	1246	А
1	Ba	1248	А
1	Ba	1250	U
1	Ba	1251	G
1	Ba	1256	А
1	Ba	1260	А
1	Ba	1266	С
1	Ba	1267	А
1	Ba	1268	G
1	Ba	1270	G
1	Ba	1274	С
1	Ba	1275	С
1	Ba	1280	G
1	Ba	1281	G
1	Ba	1282	U
1	Ba	1283	С
1	Ba	1286	G
1	Ba	1287	С
1	Ba	1288	A
1	Ba	1289	А
1	Ba	1290	A
1	Ba	1291	U
1	Ba	1292	С
1	Ba	1296	U



Mol	Chain	Res	Type
1	Ba	1297	А
1	Ba	1300	G
1	Ba	1305	U
1	Ba	1307	U
1	Ba	1308	С
1	Ba	1309	А
1	Ba	1310	G
1	Ba	1311	U
1	Ba	1312	U
1	Ba	1313	С
1	Ba	1314	G
1	Ba	1315	G
1	Ba	1319	G
1	Ba	1320	U
1	Ba	1322	G
1	Ba	1327	С
1	Ba	1329	А
1	Ba	1332	С
1	Ba	1333	G
1	Ba	1335	С
1	Ba	1336	U
1	Ba	1337	А
1	Ba	1338	С
1	Ba	1339	А
1	Ba	1341	G
1	Ba	1345	С
1	Ba	1347	G
1	Ba	1348	G
1	Ba	1356	А
1	Ba	1357	G
1	Ba	1361	U
1	Ba	1363	G
1	Ba	1368	U
1	Ba	1371	G
1	Ba	1373	A
1	Ba	1378	А
1	Ba	1380	G
1	Ba	1387	А
1	Ba	1391	U
1	Ba	1392	С
1	Ba	1393	С
1	Ba	1404	А



Mol	Chain	Res	Type
1	Ba	1408	А
1	Ba	1419	С
1	Ba	1421	С
1	Ba	1428	А
1	Ba	1429	G
1	Ba	1438	А
1	Ba	1448	G
1	Ba	1451	G
1	Ba	1456	А
1	Ba	1461	U
1	Ba	1462	U
1	Ba	1463	U
1	Ba	1464	А
1	Ba	1466	G
1	Ba	1468	G
1	Ba	1476	U
1	Ba	1483	U
1	Ba	1495	U
1	Ba	1505	G
1	Ba	1508	G
1	Ba	1510	А
1	Ba	1514	А
1	Ba	1515	G
1	Ba	1540	G
1	Ba	1541	G
1	Ba	1543	U
23	BA	11	U
23	BA	15	G
23	BA	27	G
23	BA	28	А
23	BA	34	U
23	BA	36	G
23	BA	43	A
23	BA	51	G
23	BA	52	А
23	BA	53	A
23	BA	55	G
23	BA	63	U
23	BA	70	G
23	BA	71	А
23	BA	74	U
23	BA	75	G



Mol	Chain	Res	Type
23	BA	83	G
23	BA	84	A
23	BA	90	A
23	BA	92	G
23	BA	93	U
23	BA	96	G
23	BA	101	G
23	BA	102	А
23	BA	104	С
23	BA	117	А
23	BA	119	U
23	BA	124	А
23	BA	141	U
23	BA	148	U
23	BA	149	U
23	BA	152	С
23	BA	156	А
23	BA	157	U
23	BA	158	G
23	BA	161	A
23	BA	164	А
23	BA	167	U
23	BA	168	А
23	BA	170	С
23	BA	172	U
23	BA	173	А
23	BA	177	G
23	BA	178	А
23	BA	180	G
23	BA	184	C
23	BA	185	А
23	BA	199	А
23	BA	202	A
23	BA	213	С
23	BA	215	G
$\overline{23}$	BA	216	A
23	BA	218	G
23	BA	219	A
23	BA	224	А
23	BA	225	A
23	BA	233	U
23	BA	246	U



Mol	Chain	Res	Type
23	BA	251	G
23	BA	255	G
23	BA	268	A
23	BA	269	G
23	BA	270	С
23	BA	279	А
23	BA	280	С
23	BA	285	U
23	BA	286	U
23	BA	287	G
23	BA	292	U
23	BA	293	U
23	BA	298	U
23	BA	299	U
23	BA	300	G
23	BA	301	U
23	BA	302	А
23	BA	307	A
23	BA	309	U
23	BA	310	С
23	BA	311	U
23	BA	312	А
23	BA	316	G
23	BA	320	U
23	BA	321	U
23	BA	327	G
23	BA	328	G
23	BA	333	С
23	BA	335	U
23	BA	345	С
23	BA	353	A
23	BA	365	А
23	BA	366	G
23	BA	373	А
23	BA	388	A
23	BA	389	А
23	BA	392	U
23	BA	394	U
23	BA	397	U
23	BA	402	С
23	BA	404	U
23	BA	406	А



Mol	Chain	Res	Type
23	BA	410	G
23	BA	411	А
23	BA	417	А
23	BA	432	G
23	BA	435	А
23	BA	444	С
23	BA	447	А
23	BA	449	U
23	BA	451	U
23	BA	452	G
23	BA	458	А
23	BA	460	С
23	BA	481	С
23	BA	482	U
23	BA	486	G
23	BA	490	C
23	BA	492	G
23	BA	493	А
23	BA	501	С
23	BA	502	С
23	BA	503	А
23	BA	504	G
23	BA	506	А
23	BA	512	А
23	BA	513	G
23	BA	518	А
23	BA	523	А
23	BA	527	G
23	BA	535	G
23	BA	538	G
$\overline{23}$	BA	539	G
23	BA	550	А
23	BA	553	A
$\overline{23}$	BA	554	C
23	BA	557	G
23	BA	558	A
23	BA	559	A
23	BA	563	G
23	BA	566	U
23	BA	572	С
23	BA	574	A
23	BA	576	U



Mol	Chain	Res	Type
23	BA	577	А
23	BA	578	G
23	BA	580	С
23	BA	591	А
23	BA	592	А
23	BA	594	G
23	BA	606	G
23	BA	611	U
23	BA	616	G
23	BA	617	А
23	BA	618	А
23	BA	639	U
23	BA	644	С
23	BA	645	A
23	BA	646	A
23	BA	647	G
23	BA	659	А
23	BA	672	A
23	BA	679	G
23	BA	682	А
23	BA	689	A
23	BA	690	U
23	BA	698	U
23	BA	699	U
23	BA	702	U
23	BA	713	A
23	BA	715	А
23	BA	720	A
23	BA	722	А
23	BA	730	А
23	BA	731	U
23	BA	735	С
23	BA	750	A
23	BA	754	U
23	BA	755	С
23	BA	759	U
23	BA	760	А
23	BA	761	A
23	BA	762	С
23	BA	763	A
23	BA	765	U
23	BA	766	G



Mol	Chain	Res	Type
23	BA	768	А
23	BA	771	G
23	BA	775	А
23	BA	792	U
23	BA	793	G
23	BA	797	А
23	BA	802	G
23	BA	809	А
23	BA	810	А
23	BA	816	G
23	BA	820	G
23	BA	822	G
23	BA	827	А
23	BA	829	U
23	BA	830	U
23	BA	834	А
23	BA	835	U
23	BA	836	С
23	BA	837	G
23	BA	840	С
23	BA	841	С
23	BA	842	U
23	BA	850	G
23	BA	856	U
23	BA	857	С
23	BA	868	A
23	BA	870	С
23	BA	872	U
23	BA	891	А
23	BA	892	U
23	BA	904	G
23	BA	911	А
23	BA	914	G
23	BA	918	G
23	BA	920	А
23	BA	926	G
23	BA	928	С
23	BA	940	U
23	BA	943	С
23	BA	949	С
23	BA	952	А
23	BA	955	А



Mol	Chain	Res	Type
23	BA	957	С
23	BA	960	С
23	BA	964	U
23	BA	968	А
23	BA	969	А
23	BA	970	U
23	BA	971	U
23	BA	972	А
23	BA	973	А
23	BA	975	U
23	BA	977	А
23	BA	985	А
23	BA	986	G
23	BA	988	С
23	BA	989	А
23	BA	990	G
23	BA	992	А
23	BA	997	G
23	BA	1003	А
23	BA	1005	G
23	BA	1012	G
23	BA	1018	А
23	BA	1019	А
23	BA	1024	А
23	BA	1025	А
23	BA	1027	А
23	BA	1034	А
23	BA	1040	А
23	BA	1043	U
23	BA	1047	G
23	BA	1049	С
23	BA	1056	U
23	BA	1057	A
23	BA	1066	G
23	BA	1067	U
23	BA	1069	G
23	BA	1070	А
23	BA	1076	A
23	BA	1077	U
23	BA	1078	G
$\overline{23}$	BA	1086	G
23	BA	1087	С



Mol	Chain	Res	Type
23	BA	1088	С
23	BA	1089	С
23	BA	1091	G
23	BA	1092	A
23	BA	1093	С
23	BA	1094	A
23	BA	1095	А
23	BA	1100	G
23	BA	1102	U
23	BA	1105	U
23	BA	1106	G
23	BA	1109	U
23	BA	1111	А
23	BA	1113	А
23	BA	1114	А
23	BA	1115	G
23	BA	1116	С
23	BA	1117	A
23	BA	1118	G
23	BA	1119	С
23	BA	1120	С
23	BA	1122	U
23	BA	1126	U
23	BA	1127	U
23	BA	1128	А
23	BA	1132	А
23	BA	1133	G
23	BA	1137	G
23	BA	1138	U
23	BA	1139	А
23	BA	1140	А
23	BA	1143	G
23	BA	1145	U
23	BA	1148	С
23	BA	1150	A
23	BA	1151	G
23	BA	1155	A
23	BA	1156	G
23	BA	1158	G
23	BA	1160	С
23	BA	1161	A
23	BA	1162	С



Mol	Chain	Res	Type
23	BA	1163	U
23	BA	1174	U
23	BA	1176	U
23	BA	1178	С
23	BA	1179	С
23	BA	1186	А
23	BA	1200	А
23	BA	1201	G
23	BA	1208	А
23	BA	1214	С
23	BA	1215	U
23	BA	1216	U
23	BA	1217	U
23	BA	1218	G
23	BA	1225	G
23	BA	1245	G
23	BA	1250	G
23	BA	1258	А
23	BA	1265	G
23	BA	1267	A
23	BA	1274	G
23	BA	1275	A
23	BA	1276	G
23	BA	1284	А
23	BA	1285	А
23	BA	1286	G
23	BA	1290	G
23	BA	1291	A
23	BA	1294	G
23	BA	1298	G
23	BA	1300	G
23	BA	1304	G
23	BA	1309	G
23	BA	1310	A
23	BA	1320	G
23	BA	1326	С
23	BA	1337	А
23	BA	1338	U
23	BA	1339	U
23	BA	1340	G
23	BA	1342	С
23	BA	1344	A



Mol	Chain	Res	Type
23	BA	1348	U
23	BA	1349	U
23	BA	1351	С
23	BA	1354	G
23	BA	1358	А
23	BA	1367	С
23	BA	1370	С
23	BA	1386	U
23	BA	1387	С
23	BA	1389	U
23	BA	1392	G
23	BA	1394	U
23	BA	1402	А
23	BA	1405	G
23	BA	1415	А
23	BA	1416	U
23	BA	1417	G
23	BA	1420	U
23	BA	1422	А
23	BA	1423	С
23	BA	1432	А
23	BA	1440	А
23	BA	1443	А
23	BA	1445	С
23	BA	1447	А
23	BA	1450	А
23	BA	1451	U
23	BA	1453	G
23	BA	1454	U
23	BA	1455	U
23	BA	1457	U
23	BA	1459	А
23	BA	1463	A
23	BA	1464	U
23	BA	1471	А
23	BA	1472	С
23	BA	1481	A
23	BA	1489	А
23	BA	1490	G
23	BA	1491	С
23	BA	1494	G
23	BA	1495	С



Mol	Chain	Res	Type
23	BA	1496	G
23	BA	1497	А
23	BA	1498	U
23	BA	1499	U
23	BA	1503	U
23	BA	1504	U
23	BA	1510	U
23	BA	1516	С
23	BA	1518	G
23	BA	1519	U
23	BA	1520	А
23	BA	1521	А
23	BA	1525	U
23	BA	1526	G
23	BA	1527	А
23	BA	1532	U
23	BA	1533	А
23	BA	1534	G
23	BA	1536	С
23	BA	1537	А
23	BA	1540	U
23	BA	1550	G
23	BA	1551	U
23	BA	1552	U
23	BA	1553	А
23	BA	1554	А
23	BA	1555	G
23	BA	1556	G
23	BA	1559	G
23	BA	1561	G
23	BA	1569	G
23	BA	1570	G
23	BA	1575	A
23	BA	$157\overline{6}$	A
23	BA	1578	А
23	BA	1579	С
23	BA	1580	A
23	BA	1581	U
23	BA	1582	U
23	BA	1583	G
$\overline{23}$	BA	1584	U
23	BA	1586	U



Mol	Chain	Res	Type
23	BA	1587	С
23	BA	1591	G
23	BA	1594	U
23	BA	1605	А
23	BA	1606	С
23	BA	1613	G
23	BA	1616	А
23	BA	1625	U
23	BA	1627	G
23	BA	1629	U
23	BA	1630	А
23	BA	1631	G
23	BA	1632	А
23	BA	1633	A
23	BA	1634	А
23	BA	1635	А
23	BA	1636	U
23	BA	1639	G
23	BA	1652	А
23	BA	1653	А
23	BA	1654	А
23	BA	1661	С
23	BA	1666	А
23	BA	1675	G
23	BA	1679	А
23	BA	1683	U
23	BA	1684	А
23	BA	1690	А
23	BA	1691	G
23	BA	1692	С
23	BA	1693	G
23	BA	1718	G
23	BA	1719	С
23	BA	1732	U
23	BA	1737	U
23	BA	1738	С
23	BA	1740	G
23	BA	1745	A
23	BA	1747	G
23	BA	1757	U
23	BA	1758	A
23	BA	1759	G



Mol	Chain	Res	Type
23	BA	1760	G
23	BA	1761	G
23	BA	1762	U
23	BA	1765	А
23	BA	1768	С
23	BA	1771	А
23	BA	1772	G
23	BA	1790	G
23	BA	1791	G
23	BA	1797	G
23	BA	1800	А
23	BA	1806	U
23	BA	1808	U
23	BA	1809	C
23	BA	1811	А
23	BA	1813	A
23	BA	1814	А
23	BA	1818	A
23	BA	1826	G
23	BA	1827	С
23	BA	1828	U
23	BA	1829	А
23	BA	1830	А
23	BA	1835	U
23	BA	1843	U
23	BA	1846	А
23	BA	1856	А
23	BA	1860	С
23	BA	1878	U
23	BA	1879	U
23	BA	1880	A
23	BA	1885	G
23	BA	1889	G
23	BA	1895	С
23	BA	1897	U
23	BA	1898	С
23	BA	1899	U
23	BA	1900	G
23	BA	1901	С
23	BA	1902	G
23	BA	1903	A
23	BA	1904	A



Mol	Chain	Res	Type
23	BA	1907	U
23	BA	1909	С
23	BA	1911	А
23	BA	1912	А
23	BA	1914	С
23	BA	1918	G
23	BA	1933	G
23	BA	1935	С
23	BA	1937	G
23	BA	1938	U
23	BA	1945	А
23	BA	1950	U
23	BA	1956	G
23	BA	1958	U
23	BA	1963	А
23	BA	1964	А
23	BA	1965	А
23	BA	1966	U
23	BA	1971	U
23	BA	1982	U
23	BA	1989	С
23	BA	1990	С
23	BA	1992	С
23	BA	1994	С
23	BA	1996	А
23	BA	1997	А
23	BA	1998	А
23	BA	1999	G
23	BA	2009	U
23	BA	2018	U
23	BA	2019	G
23	BA	2020	U
23	BA	2023	С
23	BA	2024	А
23	BA	2029	G
23	BA	2030	A
23	BA	2047	А
23	BA	2057	A
23	BA	2058	А
23	BA	2059	G
23	BA	2060	А
23	BA	2062	G



Mol	Chain	Res	Type
23	BA	2070	С
23	BA	2073	G
23	BA	2075	G
23	BA	2076	А
23	BA	2082	С
23	BA	2083	G
23	BA	2085	А
23	BA	2087	А
23	BA	2088	G
23	BA	2089	А
23	BA	2096	G
23	BA	2097	G
23	BA	2103	U
23	BA	2107	G
23	BA	2109	А
23	BA	2110	G
23	BA	2111	С
23	BA	2115	А
23	BA	2117	А
23	BA	2118	U
23	BA	2119	U
23	BA	2120	G
23	BA	2126	С
23	BA	2129	С
23	BA	2139	А
23	BA	2140	С
23	BA	2143	G
23	BA	2145	U
23	BA	2147	G
23	BA	2153	А
23	BA	2155	С
23	BA	2157	U
23	BA	2158	U
23	BA	2160	G
23	BA	2161	A
23	BA	2164	С
23	BA	2172	С
23	BA	2173	U
23	BA	2174	A
23	BA	2175	G
23	BA	2176	С
23	BA	2183	G



Mol	Chain	Res	Type
23	BA	2185	А
23	BA	2186	G
23	BA	2188	С
23	BA	2190	С
23	BA	2193	G
23	BA	2194	U
23	BA	2195	G
23	BA	2198	А
23	BA	2204	С
23	BA	2215	U
23	BA	2224	U
23	BA	2225	А
23	BA	2229	С
23	BA	2230	G
23	BA	2231	С
23	BA	2232	А
23	BA	2238	U
23	BA	2240	U
23	BA	2241	С
23	BA	2243	U
23	BA	2252	А
23	BA	2261	G
23	BA	2262	G
23	BA	2263	С
23	BA	2265	G
23	BA	2266	G
23	BA	2290	С
23	BA	2295	А
23	BA	2305	А
23	BA	2306	G
23	BA	2310	С
23	BA	2314	A
23	BA	$2\overline{316}$	G
23	BA	2321	С
23	BA	$2\overline{328}$	A
23	BA	2329	U
23	BA	2330	G
23	BA	2331	G
23	BA	2332	U
23	BA	$2\overline{3}33$	U
23	BA	2334	G
23	BA	2335	G



Mol	Chain	Res	Type
23	BA	2336	А
23	BA	2337	А
23	BA	2345	A
23	BA	2346	U
23	BA	2347	А
23	BA	2352	G
23	BA	2353	U
23	BA	2358	G
23	BA	2361	U
23	BA	2362	А
23	BA	2370	U
23	BA	2374	С
23	BA	2377	С
23	BA	2385	A
23	BA	2388	А
23	BA	2396	A
23	BA	2409	G
23	BA	2410	G
23	BA	2411	А
23	BA	2412	С
23	BA	2429	U
23	BA	2433	С
23	BA	2434	А
23	BA	2441	G
23	BA	2449	С
23	BA	2450	U
23	BA	2451	С
23	BA	2455	G
23	BA	2456	G
23	BA	2457	А
23	BA	2458	U
23	BA	2459	А
23	BA	2460	A
$\overline{23}$	BA	2461	A
23	BA	2462	A
23	BA	2463	G
23	BA	2468	С
23	BA	2472	G
$\overline{23}$	BA	2474	G
23	BA	2475	A
$\overline{23}$	BA	$24\overline{85}$	U
23	BA	2486	A



Mol	Chain	Res	Type
23	BA	2503	А
23	BA	2511	G
23	BA	2521	G
23	BA	2525	С
23	BA	2529	G
23	BA	2530	А
23	BA	2531	U
23	BA	2532	G
23	BA	2540	А
23	BA	2544	С
23	BA	2545	А
23	BA	2547	С
23	BA	2556	G
23	BA	2561	С
23	BA	2562	G
23	BA	2568	А
23	BA	2569	А
23	BA	2570	G
23	BA	2581	U
23	BA	2589	U
23	BA	2592	А
23	BA	2593	А
23	BA	2594	G
23	BA	2599	А
23	BA	2600	С
23	BA	2604	А
23	BA	2605	G
23	BA	2613	С
23	BA	2626	G
23	BA	2629	А
23	BA	2630	G
23	BA	2636	U
23	BA	2640	U
23	BA	2642	U
23	BA	2646	U
23	BA	2648	G
23	BA	2650	G
23	BA	2656	A
23	BA	2657	G
23	BA	2666	А
23	BA	2672	G
23	BA	2679	U



Mol	Chain	Res	Type
23	BA	2681	А
23	BA	2687	А
23	BA	2692	А
23	BA	2695	G
23	BA	2696	G
23	BA	2697	G
23	BA	2699	U
23	BA	2700	G
23	BA	2712	G
23	BA	2716	U
23	BA	2741	G
23	BA	2745	G
23	BA	2750	С
23	BA	2753	U
23	BA	2756	G
23	BA	2757	U
23	BA	2759	G
23	BA	2760	А
23	BA	2761	С
23	BA	2764	G
23	BA	2769	G
23	BA	2771	G
23	BA	2775	А
23	BA	2778	G
23	BA	2784	А
23	BA	2788	А
23	BA	2793	G
23	BA	2794	С
23	BA	2796	С
23	BA	2798	С
23	BA	2800	U
23	BA	2801	С
23	BA	2803	А
23	BA	2804	G
23	BA	2805	А
23	BA	2806	U
23	BA	2808	А
23	BA	2817	А
23	BA	2820	U
23	BA	2821	U
23	BA	2822	С
23	BA	2823	G



Mol	Chain	Res	Type
23	BA	2824	G
23	BA	2827	А
23	BA	2828	U
23	BA	2829	А
23	BA	2831	G
23	BA	2832	А
23	BA	2838	С
23	BA	2840	А
23	BA	2843	А
23	BA	2850	G
23	BA	2853	U
23	BA	2854	А
23	BA	2855	А
23	BA	2879	G
23	BA	2887	G
23	BA	2888	А
23	BA	2892	G
23	BA	2899	А
23	BA	2900	С
23	BA	2903	А
23	BA	2913	G
23	BA	2914	А
23	BA	2919	А
24	BB	10	U
24	BB	22	G
24	BB	23	U
24	BB	24	С
24	BB	33	U
24	BB	39	G
24	BB	40	С
24	BB	43	А
24	BB	51	А
24	BB	55	A
24	BB	64	А
24	BB	87	С
24	BB	88	G
24	BB	106	G
24	BB	111	С
24	BB	113	G

All (55) RNA pucker outliers are listed below:



23AA99U23AA160G23AA267G23AA268A23AA291G23AA451U23AA487U23AA513G23AA576U23AA688A23AA697U23AA697U23AA697U23AA697U23AA697U23AA1024A23AA1024A23AA1075G23AA1190A23AA1267A23AA1385G23AA2117A23AA2568A23AA2749G23AA2749G23AA267G23BA267G23BA268A23BA268A23BA268A23BA268A23BA268A23BA268A23BA268A23BA268A23BA268A23BA268A23BA268A23 <th>Mol</th> <th>Chain</th> <th>\mathbf{Res}</th> <th>Type</th>	Mol	Chain	\mathbf{Res}	Type
23AA160G23AA267G23AA268A23AA291G23AA451U23AA451U23AA513G23AA576U23AA577A23AA688A23AA697U23AA697U23AA697U23AA697U23AA1024A23AA1024A23AA1075G23AA1372C23AA1385G23AA1385G23AA2450U23AA2568A23AA2783U23AA2783U23AA267G23AA268A23AA267G23AA268A23AA267G23BA268A23BA268A23BA268A23BA267G23BA268A23BA267G23BA268A23BA268A23BA2576U23 </td <td>23</td> <td>AA</td> <td>99</td> <td>U</td>	23	AA	99	U
23AA267G23AA268A23AA291G23AA451U23AA487U23AA513G23AA576U23AA577A23AA688A23AA697U23AA697U23AA697U23AA987U23AA1024A23AA1075G23AA1190A23AA1267A23AA1372C23AA1385G23AA2450U23AA2450U23AA2783U23AA2783U23AA268A23AA267G23AA268A23AA268A23AA268A23AA267G23AA268A23AA268A23AA268A23AA268A23AA268A23AA268A23AA268A23AA268A23AA268A23 <td>23</td> <td>AA</td> <td>160</td> <td>G</td>	23	AA	160	G
23AA268A23AA291G23AA451U23AA513G23AA576U23AA577A23AA688A23AA697U23AA697U23AA697U23AA697U23AA697U23AA697U23AA987U23AA1024A23AA1075G23AA1267A23AA1385G23AA1385G23AA2450U23AA2450U23AA2783U23AA2783U23AA268A23BA267G23BA268A23BA291G23BA268A23BA267G23BA268A23BA268A23BA268A23BA268A23BA257G23BA268A23BA268A23BA268A23BA2576U23 <td>23</td> <td>AA</td> <td>267</td> <td>G</td>	23	AA	267	G
23AA291G23AA451U23AA513G23AA576U23AA577A23AA688A23AA697U23AA697U23AA697U23AA697U23AA697U23AA697U23AA987U23AA1024A23AA1075G23AA1190A23AA1372C23AA1385G23AA2450U23AA2568A23AA2749G23AA2783U23AA268A23AA268A23AA268A23AA268A23AA268A23AA268A23AA268A23BA267G23BA268A23BA268A23BA268A23BA268A23BA268A23BA268A23BA268A23BA257U23 <td>23</td> <td>AA</td> <td>268</td> <td>А</td>	23	AA	268	А
23AA451U23AA513G23AA576U23AA577A23AA688A23AA697U23AA697U23AA697U23AA697U23AA711G23AA987U23AA987U23AA1024A23AA1075G23AA1267A23AA1372C23AA1385G23AA2117A23AA2568A23AA2749G23AA2749G23BA267G23BA267G23BA268A23BA268A23BA267G23BA268A23BA267G23BA268A23BA267G23BA268A23BA267G23BA268A23BA267G23BA268A23BA267G23BA267G23BA2568A23 <td>23</td> <td>AA</td> <td>291</td> <td>G</td>	23	AA	291	G
23 AA 487 U 23 AA 513 G 23 AA 576 U 23 AA 577 A 23 AA 688 A 23 AA 697 U 23 AA 697 U 23 AA 697 U 23 AA 697 U 23 AA 987 U 23 AA 987 U 23 AA 1024 A 23 AA 1024 A 23 AA 1075 G 23 AA 1267 A 23 AA 1385 G 23 AA 1385 G 23 AA 1385 U 23 AA 2107 A 23 AA 2568 A 23 AA 2749 G 23 BA 99 U 23 </td <td>23</td> <td>AA</td> <td>451</td> <td>U</td>	23	AA	451	U
23 AA 513 G 23 AA 576 U 23 AA 577 A 23 AA 688 A 23 AA 697 U 23 AA 697 U 23 AA 697 U 23 AA 711 G 23 AA 987 U 23 AA 987 U 23 AA 1024 A 23 AA 1075 G 23 AA 1075 G 23 AA 1267 A 23 AA 1372 C 23 AA 1385 G 23 AA 1385 U 23 AA 2450 U 23 AA 2749 G 23 AA 2783 U 23 AA 2783 U 23 BA 267 G 23	23	AA	487	U
23 AA 576 U 23 AA 577 A 23 AA 688 A 23 AA 697 U 23 AA 697 U 23 AA 711 G 23 AA 840 C 23 AA 987 U 23 AA 1024 A 23 AA 1075 G 23 AA 1075 G 23 AA 1190 A 23 AA 1267 A 23 AA 1372 C 23 AA 1385 G 23 AA 1385 U 23 AA 2450 U 23 AA 2450 U 23 AA 2749 G 23 AA 2783 U 23 BA 99 U 23 BA 267 G 23	23	AA	513	G
23 AA 577 A 23 AA 688 A 23 AA 697 U 23 AA 711 G 23 AA 840 C 23 AA 987 U 23 AA 987 U 23 AA 1024 A 23 AA 1075 G 23 AA 1075 G 23 AA 1190 A 23 AA 1267 A 23 AA 1372 C 23 AA 1385 G 23 AA 1385 G 23 AA 2117 A 23 AA 2568 A 23 AA 2749 G 23 AA 2783 U 23 BA 267 G 23 BA 267 G 23 BA 268 A 2	23	AA	576	U
23 AA 688 A 23 AA 697 U 23 AA 711 G 23 AA 840 C 23 AA 987 U 23 AA 987 U 23 AA 1024 A 23 AA 1075 G 23 AA 1075 G 23 AA 1267 A 23 AA 1372 C 23 AA 1385 G 23 AA 1385 G 23 AA 1267 A 23 AA 1267 A 23 AA 1267 A 23 AA 2450 U 23 AA 2450 U 23 AA 2749 G 23 AA 2783 U 23 BA 267 G 23 BA 268 A <td< td=""><td>23</td><td>AA</td><td>577</td><td>А</td></td<>	23	AA	577	А
23 AA 697 U 23 AA 711 G 23 AA 840 C 23 AA 987 U 23 AA 1024 A 23 AA 1075 G 23 AA 1075 G 23 AA 1075 G 23 AA 1267 A 23 AA 1372 C 23 AA 1385 G 23 AA 1385 G 23 AA 1267 A 23 AA 1372 C 23 AA 1385 G 23 AA 2117 A 23 AA 2568 A 23 AA 2749 G 23 AA 2783 U 23 BA 267 G 23 BA 268 A 23 BA 268 A <t< td=""><td>23</td><td>AA</td><td>688</td><td>А</td></t<>	23	AA	688	А
23 AA 711 G 23 AA 840 C 23 AA 987 U 23 AA 1024 A 23 AA 1024 A 23 AA 1075 G 23 AA 1190 A 23 AA 1267 A 23 AA 1372 C 23 AA 1385 G 23 AA 1385 G 23 AA 1267 A 23 AA 1267 A 23 AA 1267 A 23 AA 1267 A 23 AA 2450 U 23 AA 2749 G 23 AA 2749 G 23 BA 99 U 23 BA 267 G 23 BA 268 A 23 BA 268 A <td< td=""><td>23</td><td>AA</td><td>697</td><td>U</td></td<>	23	AA	697	U
23 AA 840 C 23 AA 987 U 23 AA 1024 A 23 AA 1075 G 23 AA 1075 G 23 AA 1190 A 23 AA 1267 A 23 AA 1372 C 23 AA 1385 G 23 AA 1385 G 23 AA 1385 U 23 AA 1267 A 23 AA 1372 C 23 AA 1385 G 23 AA 2117 A 23 AA 2450 U 23 AA 2749 G 23 AA 2749 G 23 BA 160 G 23 BA 267 G 23 BA 268 A 23 BA 268 A <	23	AA	711	G
23 AA 987 U 23 AA 1024 A 23 AA 1075 G 23 AA 1190 A 23 AA 1267 A 23 AA 1372 C 23 AA 1385 G 23 AA 1385 G 23 AA 1385 G 23 AA 1267 A 23 AA 1267 A 23 AA 1372 C 23 AA 1385 G 23 AA 2450 U 23 AA 2568 A 23 AA 2749 G 23 AA 2783 U 23 BA 99 U 23 BA 267 G 23 BA 268 A 23 BA 268 A 23 BA 268 A <t< td=""><td>23</td><td>AA</td><td>840</td><td>С</td></t<>	23	AA	840	С
23 AA 1024 A 23 AA 1075 G 23 AA 1190 A 23 AA 1267 A 23 AA 1372 C 23 AA 1385 G 23 AA 1385 G 23 AA 1385 G 23 AA 1385 G 23 AA 1267 A 23 AA 1385 G 23 AA 2117 A 23 AA 2450 U 23 AA 2568 A 23 AA 2749 G 23 AA 2783 U 23 BA 99 U 23 BA 267 G 23 BA 268 A 23 BA 268 A 23 BA 268 A 23 BA 451 U <t< td=""><td>23</td><td>AA</td><td>987</td><td>U</td></t<>	23	AA	987	U
23 AA 1075 G 23 AA 1190 A 23 AA 1267 A 23 AA 1372 C 23 AA 1385 G 23 AA 1385 G 23 AA 1385 G 23 AA 1385 G 23 AA 1267 A 23 AA 1372 C 23 AA 1267 A 23 AA 2117 A 23 AA 2450 U 23 AA 2568 A 23 AA 2749 G 23 AA 2783 U 23 BA 99 U 23 BA 267 G 23 BA 268 A 23 BA 268 A 23 BA 451 U 23 BA 513 G <t< td=""><td>23</td><td>AA</td><td>1024</td><td>A</td></t<>	23	AA	1024	A
23 AA 1190 A 23 AA 1267 A 23 AA 1372 C 23 AA 1385 G 23 AA 1385 G 23 AA 1385 G 23 AA 1385 G 23 AA 1217 A 23 AA 2450 U 23 AA 2568 A 23 AA 2749 G 23 AA 2783 U 23 BA 267 G 23 BA 267 G 23 BA 268 A 23 BA 268 A 23 BA 268 A 23 BA 451 U 23 BA 451 U 23 BA 513 G 23 BA 513 G 23 BA 513 G 2	23	AA	1075	G
23 AA 1267 A 23 AA 1372 C 23 AA 1385 G 23 AA 1385 G 23 AA 1385 G 23 AA 1845 U 23 AA 2117 A 23 AA 2450 U 23 AA 2568 A 23 AA 2749 G 23 AA 2783 U 23 AA 2783 U 23 BA 267 G 23 BA 267 G 23 BA 268 A 23 BA 268 A 23 BA 268 A 23 BA 451 U 23 BA 451 U 23 BA 513 G 23 BA 513 G 23 BA 513 G	23	AA	1190	А
23 AA 1372 C 23 AA 1385 G 23 AA 1385 G 23 AA 1845 U 23 AA 2117 A 23 AA 2450 U 23 AA 2568 A 23 AA 2749 G 23 AA 2783 U 23 BA 2783 U 23 BA 267 G 23 BA 267 G 23 BA 267 G 23 BA 268 A 23 BA 268 A 23 BA 291 G 23 BA 451 U 23 BA 451 U 23 BA 513 G 23 BA 513 G 23 BA 576 U	23	AA	1267	A
23 AA 1385 G 23 AA 1845 U 23 AA 2117 A 23 AA 2450 U 23 AA 2450 U 23 AA 2568 A 23 AA 2749 G 23 AA 2783 U 23 AA 2783 U 23 BA 267 G 23 BA 267 G 23 BA 268 A 23 BA 268 A 23 BA 291 G 23 BA 451 U 23 BA 451 U 23 BA 513 G 23 BA 513 G	23	AA	1372	С
23 AA 1845 U 23 AA 2117 A 23 AA 2450 U 23 AA 2568 A 23 AA 2568 A 23 AA 2749 G 23 AA 2783 U 23 BA 2783 U 23 BA 268 A 23 BA 267 G 23 BA 268 A 23 BA 268 A 23 BA 268 A 23 BA 451 U 23 BA 451 U 23 BA 451 U 23 BA 513 G 23 BA 513 G	23	AA	1385	G
23 AA 2117 A 23 AA 2450 U 23 AA 2568 A 23 AA 2568 A 23 AA 2749 G 23 AA 2749 G 23 AA 2783 U 23 BA 267 G 23 BA 267 G 23 BA 268 A 23 BA 268 A 23 BA 268 A 23 BA 261 U 23 BA 268 A 23 BA 261 U 23 BA 261 U 23 BA 451 U 23 BA 451 U 23 BA 513 G 23 BA 576 U	23	AA	1845	U
23 AA 2450 U 23 AA 2568 A 23 AA 2749 G 23 AA 2783 U 23 AA 2783 U 23 BA 99 U 23 BA 267 G 23 BA 268 A 23 BA 268 A 23 BA 268 A 23 BA 451 U 23 BA 451 U 23 BA 513 G 23 BA 576 U	23	AA	2117	А
23 AA 2568 A 23 AA 2749 G 23 AA 2783 U 23 BA 299 U 23 BA 160 G 23 BA 267 G 23 BA 268 A 23 BA 268 A 23 BA 291 G 23 BA 451 U 23 BA 451 U 23 BA 513 G 23 BA 576 U	23	AA	2450	U
23 AA 2749 G 23 AA 2783 U 23 BA 99 U 23 BA 160 G 23 BA 267 G 23 BA 268 A 23 BA 268 A 23 BA 291 G 23 BA 451 U 23 BA 451 U 23 BA 513 G 23 BA 576 U	23	AA	2568	А
23 AA 2783 U 23 BA 99 U 23 BA 160 G 23 BA 267 G 23 BA 268 A 23 BA 268 A 23 BA 291 G 23 BA 451 U 23 BA 451 U 23 BA 513 G 23 BA 513 G	23	AA	2749	G
23 BA 99 U 23 BA 160 G 23 BA 267 G 23 BA 268 A 23 BA 268 A 23 BA 291 G 23 BA 451 U 23 BA 451 U 23 BA 513 G 23 BA 576 U	23	AA	2783	U
23 BA 160 G 23 BA 267 G 23 BA 268 A 23 BA 268 A 23 BA 291 G 23 BA 451 U 23 BA 451 G 23 BA 513 G 23 BA 513 G 23 BA 576 U	23	BA	99	U
23 BA 267 G 23 BA 268 A 23 BA 291 G 23 BA 451 U 23 BA 451 G 23 BA 513 G 23 BA 576 U	23	BA	160	G
23 BA 268 A 23 BA 291 G 23 BA 451 U 23 BA 451 G 23 BA 513 G 23 BA 576 U	23	BA	267	G
23 BA 291 G 23 BA 451 U 23 BA 487 U 23 BA 513 G 23 BA 576 U	23	BA	268	A
23 BA 451 U 23 BA 487 U 23 BA 513 G 23 BA 576 U	23	BA	291	G
23 BA 487 U 23 BA 513 G 23 BA 576 U	23	BA	451	U
23 BA 513 G 23 BA 576 U	23	BA	487	U
23 BA 576 U	23	BA	513	G
	23	BA	576	U
23 BA 577 A	23	BA	577	A
23 BA 688 A	23	BA	688	A
23 BA 697 U	23	BA	697	U
23 BA 711 G	23	BA	711	G
23 BA 840 C	23	BA	840	C
23 BA 987 U	23	BA	987	U
23 BA 1024 A	23	BA	1024	A



Mol	Chain	Res	Type
23	BA	1075	G
23	BA	1190	А
23	BA	1267	А
23	BA	1372	С
23	BA	1385	G
23	BA	1731	G
23	BA	1845	U
23	BA	2117	А
23	BA	2450	U
23	BA	2568	А
23	BA	2749	G
23	BA	2783	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
23	AA	6
23	BA	6
1	Aa	1
1	Ba	1



Continued from previous page...

Mol	Chain	Number of breaks
24	BB	1
24	AB	1
13	Am	1
13	Bm	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AA	2207:U	O3'	2208:A	Р	9.06
1	BA	2207:U	O3'	2208:A	Р	9.06
1	AA	2132:A	O3'	2133:G	Р	8.44
1	BA	2132:A	O3'	2133:G	Р	8.44
1	AA	1096:C	O3'	1097:U	Р	6.77
1	BA	1096:C	O3'	1097:U	Р	6.77
1	Aa	465:U	O3'	466:G	Р	3.97
1	Ba	465:U	O3'	466:G	Р	3.97
1	AA	1153:C	O3'	1154:G	Р	3.61
1	BA	1153:C	O3'	1154:G	Р	3.61
1	AA	1448:U	O3'	1449:A	Р	3.51
1	BA	1448:U	O3'	1449:A	Р	3.51
1	BB	114:G	O3'	115:C	Р	3.40
1	AA	2217:G	O3'	2218:G	Р	3.39
1	AB	114:G	O3'	115:C	Р	3.39
1	BA	2217:G	O3'	2218:G	Р	3.39
1	Am	93:ARG	С	94:GLY	N	3.26
1	Bm	93:ARG	С	94:GLY	N	3.26



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-3637. 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: 200



Y Index: 200



Z Index: 200

6.2.2 Raw map



X Index: 200

Y Index: 200

Z Index: 200 $\,$

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: 210



Y Index: 113



Z Index: 201

6.3.2 Raw map



X Index: 210

Y Index: 287

Z Index: 201

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


6.4 Orthogonal surface views (i)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.023. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

6.5 Mask visualisation (i)

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



7 Map analysis (i)

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

7.1 Map-value distribution (i)



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



7.2 Volume estimate (i)



The volume at the recommended contour level is 3567 $\rm nm^3;$ this corresponds to an approximate mass of 3222 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 0.148 \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 0.148 $\mathrm{\AA^{-1}}$



8.2 Resolution estimates (i)

$\begin{bmatrix} Bosolution ostimato (Å) \end{bmatrix}$	Estimation criterion (FSC cut-off)		
resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	6.76	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	10.21	16.42	10.46

*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 10.21 differs from the reported value 6.76 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-3637 and PDB model 6FXC. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.023 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 (0.023).



9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 72% 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 (0.023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	$\mathbf{Q} extsf{-score}$
All	0.7187	0.1410
A1	0.1947	0.0740
A2	0.6358	0.0860
A3	0.6434	0.0790
A4	0.7820	0.0730
AA	0.8405	0.1650
AB	0.8151	0.1500
AC	0.3935	0.0970
AD	0.5876	0.1020
AE	0.4633	0.1010
AF	0.3548	0.1100
AG	0.3846	0.1160
AH	0.6240	0.0920
AI	0.2983	0.1400
AJ	0.4468	0.0740
AK	0.5645	0.1370
AL	0.5918	0.0940
AM	0.6571	0.1060
AN	0.4773	0.1290
AO	0.7151	0.0990
AP	0.5129	0.1050
AQ	0.4952	0.0790
AR	0.6223	0.0850
AS	0.4404	0.0870
AT	0.2370	0.0990
AU	0.7098	0.1040
AV	0.3380	0.0690
AW	0.4419	0.1080
AX	0.3447	0.1120
AY	0.1168	0.1090
AZ	0.5591	0.0690
Aa	0.8309	0.1470
Ab	0.3011	0.1100
Ac	0.2628	0.1170
Ad	0.5459	0.1000

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Chain	Atom inclusion	Q-score
Ae	0.2435	0.1020
Af	0.3780	0.1040
Ag	0.2827	0.1110
Ah	0.4307	0.1020
Ai	0.4225	0.0680
Aj	0.4243	0.0600
Ak	0.4078	0.1020
Al	0.3383	0.1140
Am	0.4158	0.0890
An	0.7468	0.0700
Ao	0.5747	0.0960
Ap	0.5258	0.0830
Aq	0.4373	0.0900
Ar	0.3613	0.1070
As	0.6061	0.0900
At	0.5575	0.0980
Au	0.0646	0.0350
Av	0.2785	0.1120
B1	0.1973	0.0840
B2	0.6358	0.0930
B3	0.6434	0.0810
B4	0.7820	0.0720
BA	0.8405	0.1670
BB	0.8151	0.1460
BC	0.3930	0.0990
BD	0.5876	0.0970
BE	0.4633	0.1040
BF	0.3548	0.1090
BG	0.3846	0.1140
BH	0.6231	0.0910
BI	0.2983	0.1420
BJ	0.4468	0.0790
BK	0.5645	0.1350
BL	0.5929	0.0930
BM	0.6559	0.1100
BN	0.4761	0.1250
BO	0.7151	0.0970
BP	0.5129	0.1060
BQ	0.4952	0.0760
BR	0.6209	0.0870
BS	0.4404	0.0890
BT	0.2370	0.0930

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Chain	Atom inclusion	Q-score
BU	0.7098	0.0990
BV	0.3380	0.0710
BW	0.4400	0.1140
BX	0.3447	0.1090
BY	0.1168	0.1110
BZ	0.5591	0.0670
Ba	0.8308	0.1470
Bb	0.3011	0.1110
Bc	0.2628	0.1140
Bd	0.5466	0.1000
Be	0.2435	0.0970
Bf	0.3780	0.1110
Bg	0.2836	0.1120
Bh	0.4307	0.0990
Bi	0.4236	0.0750
Bj	0.4229	0.0550
Bk	0.4078	0.1060
Bl	0.3383	0.1140
Bm	0.4158	0.0920
Bn	0.7468	0.0610
Bo	0.5747	0.0980
Bp	0.5258	0.0890
Bq	0.4356	0.0940
Br	0.3613	0.1120
Bs	0.6061	0.0860
Bt	0.5575	0.0990
Bu	0.0646	0.0430
Bv	0.2785	0.1120

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